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Code_Saturne documentation

Code_Saturne version 1.3.2 practical user's guide

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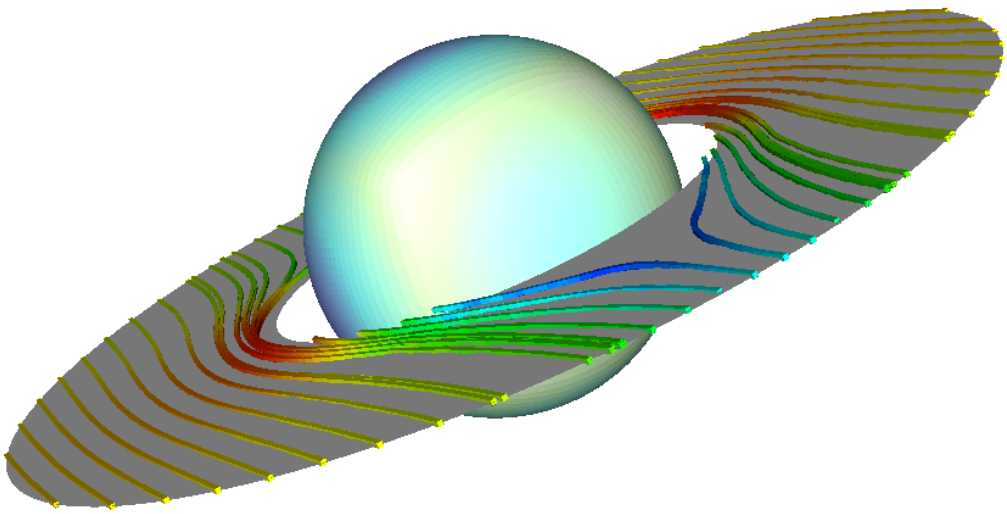

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ABSTRACT

Code_Saturne is a system designed to solve the Navier-Stokes equations in the cases of 2D, 2D axisymmetric or 3D flows. Its main module is designed for the simulation of flows which may be steady or unsteady, laminar or turbulent, incompressible or potentially dilatable, isothermal or not. Scalars and turbulent fluctuations of scalars can be taken into account. The code includes specific modules, referred to as "specific physics", for the treatment of lagrangian particle tracking, semi-transparent radiative transfer, gas combustion, pulverised coal combustion, electricity effects (Joule effect and electric arcs) and compressible flows. The code also includes an engineering module, Matisse, for the simulation of nuclear waste surface storage.
Code_Saturne relies on a finite volume discretisation and allows the use of various mesh types which may be hybrid (containing several kinds of elements) and may have structural non-conformities (hanging nodes).

The present document is a practical user's guide for *Code_Saturne* version 1.3.2. It is the result of the joint effort of all the members in the development team. It presents all the necessary elements to run a calculation with *Code_Saturne* version 1.3.2. It then lists all the variables of the code which may be useful for more advanced utilisation. The user subroutines of all the modules within the code are then documented. Eventually, for each key word and user-modifiable parameter in the code, their definition, allowed values, default values and conditions for use are given. These key words and parameters are grouped under headings based on their function. An alphabetical index list is also given at the end of the document for easier consultation.

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1 Introduction

Code_Saturne is a system designed to solve the Navier-Stokes equations in the cases of 2D, 2D axisymmetric or 3D flows. Its main module is designed for the simulation of flows which may be steady or unsteady, laminar or turbulent, incompressible or potentially dilatable, isothermal or not. Scalars and turbulent fluctuations of scalars can be taken into account. The code includes specific modules, referred to as "specific physics", for the treatment of lagrangian particle tracking, semi-transparent radiative transfer, gas combustion, pulverised coal combustion, electricity effects (Joule effect and electric arcs) and compressible flows. The code also includes an engineering module, Matisse, for the simulation of nuclear waste surface storage.

Code_Saturne is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version. *Code_Saturne* is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.[1]

Code_Saturne relies on a finite volume discretisation and allows the use of various mesh types which may be hybrid (containing several kinds of elements) and may have structural non-conformities (hanging nodes).

Code_Saturne is composed of two main elements :

- the Kernel module is the numerical solver
- the Preprocessor module is in charge of mesh data reading (many file formats allowed), mesh pasting (arbitrary interfaces), domain decomposition for parallel computing and definition of periodicity boundary conditions (translation and/or rotation)

Code_Saturne also relies on two compulsory libraries (under LGPL licence) :

- BFT (Base Functions and Types) for the management of memory and input/output as well as specific utilities (estimation of time and memory usage for instance)
- FVM (Finite Volume Mesh) for the post-processing output and the management of code coupling

The present document is a practical user's guide for *Code_Saturne* version 1.3.2. It is the result of the joint effort of all the members in the development team.

The aim of this document is to give practical information to the users of *Code_Saturne*. It is therefore strictly oriented towards the usage of the code. For more details about the algorithms and their numerical implementation, please refer to the reports [10] and [3], and to the theoretical documentation [11], which is newer and more detailled (the latest updated version of this document is available on-line with the version of *Code_Saturne* and accessible through the command `info_cs noyau`).

The present document first presents all the necessary elements to run a calculation with *Code_Saturne* version 1.3.2. It then lists all the variables of the code which may be useful for more advanced utilisation. The user subroutines of all the modules within the code are then documented. Eventually, for each key word and user-modifiable parameter in the code, their definition, allowed values, default values and conditions for use are given. These key words and parameters are grouped under headings based on their function. An alphabetical index list is also given at the end of the document for easier consultation.

[1] You should have received a copy of the GNU General Public License along with *Code_Saturne*; if not, write to the Free Software Foundation, Inc., 51 Franklin St, Fifth Floor, Boston, MA 02110-1301 USA

2 Practical information about *Code_Saturne*

2.1 System Environment for *Code_Saturne*

2.1.1 Preliminary settings

At the install procedure of *Code_Saturne*, a directory is dedicated to the code and its components. It is stored in the environment variable `PATHCS`. It is usually the root of a specific account `/home/saturne`. For installs outside EDF R&D, please refer to the administrator who installed the code for the `PATHCS` location.

The current version of *Code_Saturne* (1.3.2) is located in the directory `$PATHCS/Noyau/ncs-1.3.2` .

In order to use *Code_Saturne*, every user must add the following line in their file "`.profile`"[2]:

. `xxxxxxx/Noyau/ncs-1.3.2/bin/cs_profile`, where `xxxxxxx` represents the PATHCS directory where *Code_Saturne* and its components have been installed (refer to the administrator responsible for *Code_Saturne*).

This command runs the environment file of *Code_Saturne*, which sets the different environment variables to their correct value. ***Code_Saturne* will not work correctly if those variables have not been set properly**.
After adding this line to the `.profile`, it is necessary to logout of the session and relog in (simply reading the file by typing "`. ~/.profile`" is usually not enough and might not set the `PATH` variable correctly for the whole session).

WARNING: Other pieces of information related to Code_Saturne must not be included in `.profile`. In particular, lines referring to previous versions of the code must be suppressed

2.1.2 Standard architecture of the directories

The standard architecture for the simulation studies is:

A study directory containing:

- A directory `MAILLAGE` containing the mesh(es) necessary for the study
- A directory `POST` for the potential post-processing routines (not used directly by the code)
- One or several calculation directories

Every calculation directory contains:

- A directory `FORT` for the potential user subroutines necessary for the calculation
- A directory `DATA` for the calculation data (data file from the interface, input profiles, thermochemical data, ...)
- A directory `SCRIPTS` for the launch script
- A directory `RESU` for the results
  To improve the calculation traceability, the files and directories sent to `RESU` after a calculation are given a suffix identifying the calculation start date and time by an eight-digit number (two digits for each month, day, hour and minute; the result of a calculation started at 14h03 on december 31st will therefore be indexed 12311403)

[2] or `.monprofile` if the modifications of the `.profile` file are reserved for the administators, as is the case in the MFEE departement of EDF

In the standard cases, `RESU` contains a directory `CHR.ENSIGHT.mmddhhmm` with the post-processing files in *EnSight* format, a directory `SUITE.mmddhhmm` for the calculation restart files, a directory `HIST.mmddhhmm` for the files of chronological record of the results at specific locations (probes), `listpre.mmddhhmm` and `listing.mmddhhmm` files reporting the Preprocessor and the Kernel execution. For an easier follow-up of the modifications in former calculations, the user-subroutines used in a calculation are stored in a directory `FORT.mmddhhmm` in the directory `RESU`. The *Xml* Interface data file, thermo-chemical data files and launch script are also copied into the directory `RESU` with the appropriate suffix (whatever its name, the launch script appears in the directory `RESU` as `lance.mmddhhmm`). `compil.log.mmddhhmm` and `resume.mmddhhmm` are respectively reports of the compilation phase and general information on the calculation (which kind of machine, which user, which version of the code, ...). Eventually, when the user subroutines produce specific result files (extraction of 1D profiles for instance), a directory `RES_USERS.mmddhhmm` is created in the directory `RESU` for these files[3].

During calcualtions coupled with SYRTHES (option specified in the launch script of *Code_Saturne* or *via* the Interface) the same organisation is used for the files related to *Code_Saturne*. For the files related to SYRTHES, the localisation of the upstream files is specified in the `syrthes.env` file. Yet, the launch script is built presuming that the following organisation is applied:

- a directory `FORT_SYR` for the potential SYRTHES user subroutines
- a directory `DATA_SYR` containing the configuration file `syrthes.env` (localisation of files specific to SYRTHES). The file defining the SYRTHES calculation options (`syrthes.data`) and the potential restart files can also be placed in this directory.

The SYRTHES result files (geometry file, chronological result files, calculation restart files and the historic file) are placed in a sub-directory `RESU_SYR.mmddhhmm` of the `RESU` directory, where `mmddhhmm` corresponds to the calculation identification suffix.

The SYRTHES execution report file is placed in the `RESU` directory (same as for the *Code_Saturne* review) under the name `listsyr.mmddhhmm`. The compilation report file is the same for SYRTHES and *Code_Saturne*. It is placed in the `RESU` directory under the name `compil.log.mmddhhmm`. For an easier follow-up of the modifications in former calculations, the potential SYRTHES user-subroutines used in a calculation are stored in a directory `FORT_SYR.mmddhhmm` in the directory `RESU`.

[3] in order for the script to copy them properly, their names have to be given in the variable `FICHIERS_RESULTATS_UTILISATEUR` of the launch script, see §2.6

Below are typical contents of a case directory CASE1 in a study STUDY (*Code_Saturne* calculation coupled with SYRTHES):

`STUDY/CASE1/DATA:`	***Code_Saturne* data**
`SaturneGUI`	Graphical User Interface launch script
`study.xml`	Graphical User Interface parameter file
`THCH`	example of thermochemical files (used with the specific physics modules for gas combustion, pulverised coal or electric arcs)
`STUDY/CASE1/DATA_SYR:`	**SYRTHES data**
`syrthes.data`	SYRTHES data file
`syrthes.env`	SYRTHES configuration file
`STUDY/CASE1/FORT:`	***Code_Saturne* user subroutines**
`USERS`	examples of a user subroutines
`usclim.F`	user subroutines used for the present the calculation
`usini1.F`	
`STUDY/CASE1/RESU:`	**results**
`CHR.ENSIGHT.08211921`	directory containing the *Code_Saturne* post-processing results in the *EnSight* format for the calculation 08211921 (contains both volume and boundary results; the contents of the directory are user modifiable)
`FORT.08211921`	*Code_Saturne* user subroutines used for the calculation 08211921
`FORT_SYR.08211921`	SYRTHES user subroutines used in the calculation 08211921
`HIST.08211921`	directory containing the chronological records for *Code_Saturne*
`RES_USERS.08211921`	optional directroy containing the user results files
`SUITE.08211921`	directory containing the *Code_Saturne* restart files
`compil.log.08211921`	compilation report
`study.xml.08211921`	Graphical User Interface parameter file used for the calculation 08211921
`lance.08211921`	launch script used for the calculation 08211921 (whatever the name given to the file in the `SCRIPT` directory, the file will be referred as "`lance.*`" in the `RESU` directory)
`listpre.08211921`	execution report for the Preprocessor module of *Code_Saturne*
`listing.08211921`	execution report for the Kernel module of *Code_Saturne*
`listsyr.08211921`	execution report for SYRTHES
`resume.08211921`	general information (machine, user, version, ...)
`RESU_SYR.08211921:`	**SYRTHES results (file names given in the `syrthes.env` file)**
`geoms`	SYRTHES solid geometry file
`histos1`	SYRTHES chronological records at specified probes
`resus1`	SYRTHES calculation restart file (1 time step)
`resusc1`	SYRTHES chronolgical solid post-processing file (may be tranformed into the *EnSight* format with the *syrthes2ensight* utility)
`STUDY/CASE1/SCRIPTS:`	**launch script**
`lance`	launch script (compliant with all architectures on which *Code_Saturne* has been ported)

2.1.3 *Code_Saturne* Kernel library files

Below are given information about the content of the *Code_Saturne* base directories. They are not of vital interest for the user, but given only as general information. Indeed, the case preparer `cree_sat` automatically extracts the necessary files and prepares the launch script without the user having to go directly into the *Code_Saturne* base directories (see §2.3). The `info_cs` gives direct access to the most needed information (especially the user and progammer's guides and the tutorial) without the user having to look for them in the *Code_Saturne* directories.

The subdirectory `arch` contains the libraries and compiled executables.

The environment variable `NOM_ARCH` allows to distinguish the different architectures:

- `Blue_Gene_L` for the EDF BlueGene machine
- `HP-UX` for HP-UX system
- `IRIX64` for SGI Irix system
- `Linux` for general PC machines under Linux
- `Linux_CCRT` Opteron cluster (Tantale cluster at CCRT)
- `Linux_Ch` for the Chatou cluster
- `Linux_IA64` for Itanium clusters (Platine cluster at the CCRT)
- `SunOS` for Sun machines

For each architecture, a subdirectory (named after `NOM_ARCH`) stores the compiled elements (`libsaturne*.a` libraries in `lib` and executable in `bin`[4]). The launch script automatically loads them for the standard calculations. The different libraries correspond to the different modules of *Code_Saturne*:

- `libsaturneBASE.a` for the basic Kernel,
- `libsaturneCOGZ.a` for the gas combustion module,
- `libsaturneCFBL.a` for the compressible module,
- `libsaturneCPLV.a` for the pulverised coal combustion module,
- `libsaturneELEC.a` for the electric module,
- `libsaturneFUEL.a` for the heavy fuel oil combustion module,
- `libsaturneLAGR.a` for the lagrangian module,
- `libsaturneMATI.a` for the Matisse module,
- `libsaturneRAYT.a` for the radiation module.

Different compilation options are available for each module:

- DBG for debugging,
- EF for the "Electric Fence" utility,
- LO for low optimisation,
- PROF for profiling,

[4] This executable is used only for standalone mesh analysis. In a standard *Code_Saturne* run, the executable is recompiled to allow for user routines to be taken into account.

- PUR to use the "Purify" utility.

Each option is related to a specific library, for instance `libstaurneBASELO.a` for the "low optimisation" library of the base module.

The data files (for instance thermochemical data) are located in the directory `data`.

The source files, when available, are stored in the directory `src`, under subdirectories corresponding to each module: `base` (general routines), `cfbl` (compressible flows), `cogz` (gas combustion), `cplv` (pulverised coal combustion), `elec` (electric module), `fuel` (heavy fuel oil combustion module), `lagr` (lagrangian module, `mati` (Matisse module), `pprt` (general specific physics routines) and `rayt` (radiative heat transfer).

The user subroutines are available in the directory `users`, under similar subdirectories corresponding to each module: `base`, `cfbl`, `cogz`, `cplv`, `elec`, `fuel`, `lagr`, `pprt` and `rayt`. The case preparer `cree_sat` copies all these files in the user directory `FORT/USERS` during the case preparation.

The "include" files are available in the directory `include`, under similar subdirectories corresponding to each module: `base`, `cfbl`, `cogz`, `cplv`, `elec`, `fuel`, `lagr`, `mati`, `pprt` and `rayt`.

The directory `bin` contains an example of the launch script, the compilation parameter files and various utility programs.

2.2 Setting up and running of a calculation

2.2.1 Step by step calculation

This paragraph summarises the different steps which are necessary to prepare and run a standard case:

- Check the version of *Code_Saturne* set for use in the environment variables (`info_cs version`). If it does not correspond to the desired version, update the `.profile` file to set the environment variables correctly. Log out of the session and log in again to take the modifications into account properly (cf. §2.1.1).
- Prepare the different directories using `cree_sat`(see §2.3) and, when needed, add the directories `DATA_SYR` and `FORT_SYR` which are required to accomodate the SYRTHES files.
- Place the mesh(es) in the directory `MAILLAGE`. Make sure they are in a format compliant with *Code_Saturne* (see §2.4.1). There can be several meshes in case of mesh pasting or coupling with SYRTHES [5].
- Go to the directory `DATA` and launch the Graphical User Interface using the command `./SaturneGUI` (see §2.7).
- Place the necessary user subroutines in the directory `FORT` (see §4). When not using the Interface, some subroutines are compulsory.

  For the standard physics:

  compulsory without Graphical User Interface:
  - `usini1` to specify the calculation parameters
  - `usclim` to manage the boundary conditions

  very useful:
  - `usphyv` to manage the variable physical properties (fluid density, viscosity ...)
  - `usiniv` to manage the non-standard initialisations

  For the specific physics "gas combustion":
  (not compliant with the Graphical User Interface in version 1.3.2)

[5] SYRTHES uses meshes composed of 10-node tetrahedra (vertices and centers of edges)

compulsory:

- `usini1` to specify the calculation parameters
- `usppmo` to select a specific physics module and combustion model
- `usebuc`, `usd3pc` or `uslwcc` (depending on the selected combustion model) to manage the boundary conditions of *all variables* (*i.e.* not only the ones related to the combustion model)

very useful:

- `usebu1`, `usd3p1` or `uslwc1` (depending on the selected combustion model) to specify the calculation options for the variables corresponding to combustion model
- `usebui`, `usd3pi` or `uslwci` (depending on the selected combustion model) to manage the initialisation of the variables corresponding to the combustion model

For the specific physics "coal combustion":

compulsory without Graphical User Interface:

- `usini1` to specify the calculation parameters
- `usppmo` to select the specific physics module
- `uscpcl` or `uscplc` (depending on the specific physics module) to manage the boundary conditions of *all variables* (*i.e.* not only the ones related to the specific physics module)

very useful:

- `uscpi1` to specify the calculation options for the variables corresponding to the specific physics module
- `uscpiv` to manage the initialisation of the variables corresponding to the specific physics module

For the specific physics "electric module" (Joule effect and electric arc):
(not compliant with the Graphical User Interface in version 1.3.2)

compulsory:

- `usini1` to specify the calculation parameters
- `usppmo` to select the specific physics module
- `uselcl` to manage the boundary conditions of *all variables* (*i.e.* not only the ones related to the electric module)
- `useliv` to initialise the enthalpy in case of Joule effect
- `uselph` to define the physical properties in case of Joule effect

very useful:

- `useli1` to manage the options related to the variables corresponding to the electric module
- `useliv` to manage the initialisation of the variables corresponding to the electric module

For the specific physics "heavy fuel oil combustion module":)
(not compliant with the Graphical User Interface in version 1.3.2)

compulsory:

- `usini1` to specify the calculation parameters
- `usppmo` to select the specific physics module
- `usfucl` to manage the boundary conditions of *all variables* (*i.e.* not only the ones related to the specific physics module)

very useful:

- `usfui1` to specify the calculation options for the variables corresponding to the specific physics module
- `usfuiv` to manage the initialisation of the variables corresponding to the specific physics module

For the Lagrangian module (dispersed phase):

(the continuous phase is managed in the same way as for a case of standard physics)
(the Lagrangian module is not compliant with the Graphical User Interface in version 1.3.2)

compulsory:

- `uslag1` to manage the calculation conditions
- `uslag2` to manage the boundary conditions for the dispersed phase

very useful:

- `uslabo` to manage potential specific treatments at the boundaries (rebound conditions, specific statistics, ...)

For the compressible module:

(not compliant with the Graphical User Interface in version 1.3.2)

compulsory:

- `uscfx1` et `uscfx2` to manage the calculation parameters
- `uscfcl` to manage the boundary conditions
- `uscfth` to define the thermodynamics.

very useful:

- `uscfxi` to manage non-standard initialisations of the variables

The comprehensive list of the user subroutines and their instructions for use are given in §4.

- If necessary, place in the directory `DATA` the different external data (input profiles, thermochemical data files, ...)
- Prepare the launch script `lance`, directly or through the Graphical Interface (see §2.6)
- Run the calculation and analyse the results
- Purge the temporary files (in the directory `RUN` defined in the launch script, see §2.6)

2.2.2 Temporary execution directory

During a calculation, *Code_Saturne* uses a temporary directory for the compilation and the execution, the result files being only copied at the end in the directory `RESU`. This temporary directory is defined in the variable `RUN` of the launch script. This variable is set top a default value in the non-user section of the launch script, depending on the architecture:
`RUN=$HOME/tmp_Saturne/$ETUDE/$CAS.mmddhhmm` for stand-alone workstations or for the Chatou cluster
`RUN=$SCRATCHDIR/tmp_Saturne/$ETUDE/$CAS.mmddhhmm` for Tantale and Platine at the CCRT
where `$ETUDE` and `$CAS` are the names of the study and the case. The usual suffix with the date and time is added so that successive calculations will not get mixed-up.

This default value might not always be the optimal choice. Indeed, on a stand-alone machine, it might be useful to take advantage of large sized local disks on a machine when the `$HOME` account is on an NFS disk.

For this matter, the variable `CS_TMP_PREFIX` of the launch script (see §2.6) allows the user to change this directory. If the variable is empty, the default `RUN` directory will be used. If it is not empty, the launch script will set the `RUN` directory to `$CS_TMP_PREFIX/tmp_Saturne/$ETUDE/$CAS.mmddhhmm`.

WARNING: in most cases, the temporary directories are not deleted after a calculation. They will accumulate and may hinder the correct running of the machine.

It is therefore essential to remove them regularly.

2.2.3 Execution modes

As explained before, *Code_Saturne* is composed of two modules, the Preprocessor and the Kernel. The Preprocessor is in charge of the preprocessing. It reads the meshes and performs the necessary pastings and domain decompositions. The resulting data are transfered to the Kernel through specific files, one for each processor the Kernel will be running on. These files are named `n00001` to `n`N, N being the number of processors used for the calculation, and stored in a subdirectory `preprocessor_output` of the temporary execution directory. In a standard calculation, the files are left there as they have no interest for data analysis and are too dependent on the number of processors or the machine to be kept.

Yet, the Preprocessor module does not work in parallel and sometimes requires a large amount of memory. Hence it is sometimes useful to run the Preprocessor separately, on a machine or in batch queues with extended memory, and to run the proper parallel calculation on another machine or in another batch queue. The launch scripts therefore defines three "execution modes", that can be specified in the variable `MODE_EXEC` (see §2.6):

`complet`: complete mode. The Preprocessor module is executed for preprocessing, followed by the Kernel for the calculation. The `preprocessor_output/n*` files are created and left in the temporary execution directory.

`pre-traitement`: only the Preprocessor module is executed. The `preprocessor_output/n*` files are stored in a directory `PRE_TRAITEMENT.mmddhhmm` automatically created in the `RESU` directory, for later use.

`calcul`: only the Kernel is executed. The `preprocessor_output/n*` files are read from the directory specified in the variable `PRE_TRAITEMENT_AMONT` of the launch script.

2.2.4 Interactive modification of the target time step

During a calculation, it is possible to change the limit time step number (NTMABS) specified through the Interface or in `usini1`. To do so, a file named `ficstp` must be placed in the temporary execution directory (see §2.2.2). This file must contain a blank first line and the second line indicating the value of the new limit number of time steps.
If this new limit has already been passed in the calculation, *Code_Saturne* will stop properly at the end of the current time step (the results and restart files will be written correctly).
This procedure allows the user to stop a calculation in a clean and interactive way whenever they wish.

2.3 Case preparer

The case preparer `cree_sat` automatically creates a study directory according to the typical architecture and copies and pre-fills an example of calculation launch script.

The syntax of `cree_sat` is as follows:

`cree_sat -etude STUDY CASE_NAME1 CASE_NAME2...`
creates a study directory `STUDY` with case subdirectories `CASE_NAME1` and `CASE_NAME2`... If no case name is given, a default case directory called `CAS1` is created.

`cree_sat -cas DEBIT3 DEBIT4`
executed in the directory `STUDY` adds the case directories `DEBIT3` and `DEBIT4`.

An option `-noihm` is available for the use of *Code_Saturne* without Graphic Interface (see §2.7). This option must be either the first or the last argument and appear only once.

In the directory `DATA`, `cree_sat` places a subdirectory `THCH` containing examples of thermochemical data files used for pulverised coal combustion, gas combustion or electric arc. The file to be used for the calculation must be copied directly in the `DATA` directory and its name must be referenced in the launch script in the variable DONNEES_THERMOCHIMIE. All other files in the `DATA` or in the `THCH` will be ignored.

`cree_sat` also places in the directory `DATA` the launch script for the Graphical User Interface: `SaturneGUI`.

In the directory `FORT`, `cree_sat` creates a subdirectory `USERS` containing all the user subroutines, classified by module type: `base`, `cfbl`, `cogz`, `cplv`, `elec`, `fuel`, `lagr`, `pprt` and `rayt`. Only the user subroutines placed directly under the directory `FORT` will be considered. The others will be ignored.

In the directory `SCRIPTS`, `cree_sat` copies and pre-fills an example of the launch script: `lance`. The study, case and user name are filled automatically in the launch script, as are the paths leading to the different directories. Other parameters must be specified in the script (see §2.6), especially the mesh file(s) to use (by default a name `$ETUDE.unv` is put), but everything can be specified throuhg the Graphical Interface.

2.4 Preprocessing

The Preprocessor module of *Code_Saturne* is in charge of the preprocessing. It reads the mesh file(s) (under any supported format) and transfers the necessary information to the Kernel. Mesh pasting and domain decomposition for parallel calculations are made during this phase. In case of periodic boundary conditions, the Preprocessor module also identifies the boundary faces that are related through periodicity and creates the corresponding connectivity table.

For a complete information on the Preprocessor module, please refer to the corresponding user's guide [9] (available on-line through the command `info_cs ecsmu`).

2.4.1 Usable meshes

Code_Saturne allows to run calculations using meshes of different formats:

- I-deas universal (`*.unv`) format, generated by I-deas (Master Series 6 to 9, NX series 10 to 12), ICEM, ...

- SIMAIL NOPO format: the `*.des` files may be read directly by *Code_Saturne*.

- NUMECA Hex format (`*.hex` files): this format is seldom used. It is the product of *IggHexa* (which has since become *Hexpress*). It is not maintained, since the corresponding mesh generator in not available at EDF R&D/MFEE. The filter is based on specifications and some example meshes provided by the NUMECA company in 2001.

- MED 2.3. format: this format used by the SALOME platform and many EDF and CEA tools is based on HDF5 files.

- CGNS 2.0 (or later) format: CFD General Notation System format, used extensively by NASA, Boeing, ONERA, and ICEM (preferred over I-deas universal format for files generated with ICEM, as it may handle more cell types and leads to smaller files).

- EnSight 6 or later and EnSight Gold format. Note that EnSight 6 format files generated by Harpoon have badly-oriented prism type cells, and require the using the `-reorient` Preprocessor option.

- Gmsh format (free 3D mesh generation tool with integrated pre- and post-processing functions).

- Comet-Design pro-STAR/STAR4 format (polyhedric mesh generation tool). This might allow reading of files generated by pro-STAR, though it has only been tested on polyhedral meshes generated by Comet-Design (now STAR-Design).

- Gambit Neutral format: format of the FLUENT mesh generator.

The use of files of the "Common Solver" type[6] is still possible but is not maintained anymore. The reading of the mesh is done directly from the Kernel, without the Preprocessor module. The variable SOLCOM must be set to 1 in the launch scripts. Many potentialities of *Code_Saturne* are not compliant with this file format (mesh pasting with hanging nodes, periodicity, parallel computing, ...). The `slc2ideas` utility can be used to convert the 'Common Solver' files to the I-deas format. `slc2ideas` is automatically available in the user's PATH (who can therefore enter the command `slc2ideas` directly) when the environment variables for *Code_Saturne* have been set correctly. However, not all the files can be converted. In particular, they must comply with the initial choice (`tlc`) according to which each internal face possesses two and only two neighboring cells, and each boundary face only one neighboring cell. For non-converted, or non-convertale meshes of the 'Common Solver' type, the calculation must be done without using the Preprocessor (keyword SOLCOM=1). For all the other formats, the Preprocessor must be used (SOLCOM=0).

The Preprocessor can also accept zipped mesh files (for Formats other than MED or CGNS, which use specific external libraries) on most machines.

WARNING: Unless a specific option is used, the Preprocessor module determines the mesh format directly from the file suffix: *".unv"* for the universal Ideas format, *".des"* for the SIMAIL format, *".hex"* fot the NUMECA Hex format, *".med"* for the MED format, *".cgns"* for the CGNS format, *".case"* for the EnSight format, *".ngeom"* for the Comet format, *".msh"* for the Gmsh format, *".neu"* for the Gambit Neutral format, (voir `info_cs ecsmu`).

WARNING: Some turbulence models ($k-\varepsilon$, $R_{ij}-\varepsilon$ SSG, ...) used in *Code_Saturne* are "High-Reynolds" models. Therefore the size of the cells neighboring the wall needs to be greater than the thickness of the viscous sublayer (at the wall, $y^+ > 2.5$ is required, and $30 < y^+ < 100$ is preferable). If the mesh does not match this constraint, the results may be false (particularly if thermal phenomena are involved). For more details on these constraints, see the keyword `ITURB`.

2.4.2 Preprocessor command line options

A complete description of the Preprocessor command line options can be found in [9], accessible by the command `info_cs ecsmu`. The executable of the Preprocessor module is `ecs`, accessible directly once the environment variables of *Code_Saturne* are set properly. A summary of the command line options is also given by the command `ecs -help`.

For the main options, the launch script `lance` contains corresponding environment variables at its beginning, that are used later when the executable is called. This way, the user only has to fill these variables and doesn't need to search deep in the script for the Preprocessor command line.

The main options are:

- `-help`: gives a summary of the different command line options
- `-m mesh1 mesh2`: used to specify the names of the different meshes used. The launch script automatically calls the Preprocessor with the option `-m $MAILLAGE`, where `MAILLAGE` is the variable where the user has specified the different meshes to be used.
- `-p n`: to trigger the decomposition of the domain into `n` subdomains, for parallel computing. In the launch script, the number of processors used is specified in the `NOMBRE_DE_PROCESSEURS` variable, or through the batch headers. If necessary, the launch script then automatically passes the `-p` option to the Preprocessor command line (see 2.6).
- `-join`: triggers the mesh pasting functions. If nothing more is specified, every area of contact between two meshes will be pasted together. The pasting can be limited to certain selected faces. For instance, to paste only the faces of colors 6 and 7, the full option will be `-rc -color 6 7`.

[6] File type specifically developped for the early prototype versions of *Code_Saturne* to be read directly by the Kernel while the Preprocessor module was under development (extension `tlc`)

These options are to be specified in the `COMMANDE_RC` variable in the launch script, to be automatically passed to the command line.

- `-perio`: triggers periodic boundary conditions. Two types of periodic boundaries are possible: translation or rotation (see §3.7 for additional details). For the translation, the basic option line is `-perio -trans tx ty tz`
  where `tx`, `ty` and `tz` are the coordinates of the translation vector. For the rotation, there are two possibilities. The transformation can be defined with a rotation angle (in degrees, between -180 and 180), a direction and an invariant point
  `-perio -rota -angle a -dir dx dy dz -invpt px py pz`
  (with obvious notations), or by giving the rotation matrix and an invariant point
  `-perio -rota -matrix m11 m12 m13 m21 m22 m23 m31 m32 m33 -invpt px py pz`
  A rotation and a translation can be combined, by giving both `-rota` and `-trans` specifications. The translation will always be applied first, whatever the order in which the rotation and the translation have been given.
  The orientation of the transformations is not important since both the transformation and its inverse will be used to connect faces. Yet, when combining a translation and a rotation, the orientations given for both have to be consistent.
  It is possible (and usually recommended) to restrict the search for periodic connections between faces to a certain group of faces, by adding selection arguments like `-color`. It is also possible to specify up to 3 independent periodicities, simply by repeating the `-perio` option. Below is given a example of the option line for a triple periodicity (the `\` indicates the continuation of the command line):
  ```
  -perio -trans -10.2 0 0 -color 2 \
  -perio -rota -angle 90 -dir 0 0 1 -invpt 0 0 0 -color 3 4 \
  -perio -trans 0 1 0 -rota -matrix 1 0 0 0 0 -1 0 1 0 -invpt 0 0 -0.2
  ```
  This option is to be specified in the `COMMANDE_PERIO` variable in the launch script, to be automatically passed to the command line.

- `-reorient`: try to re-orient badly-oriented cells if it is necessary to compensate for mesh-generation software whose output does not conform to the format specifications.

2.5 Kernel command line options

In the standard cases, the compilation of *Code_Saturne* and its execution are entirely controlled by the launch script. The potential command line options are passed through user modifiable variables at the beginning of the script. This way, the user only has to fill these variables and doesn't need to search deep in the script for the Kernel command line. Yet, below is given the complete list of options, with the variables in which they should be specified in the script.

- `-ec n` or `--echo-comm n`: triggers the display of the communications between the Preprocessor module and the Kernel.
  `n=-1`: display only the error messages
  `n=0`: display the headers of messages
  `n>0`: display the headers and the n first and last elements of the messages
  The usage of this option is very limited, and generally restricted to developpers. The value of `n` is to be placed in the `ECHOCOMM` variable of the launch script, the option `--echo-comm $ECHOCOMM` is then automatically passed to the Kernel command line.

- `-solcom`: this option indicates that the Kernel will read the mesh directly, not using the Preprocessor output files. This is only possible with "Common Solver" type of mesh files (see §2.4.1 for restrictions).
  This option is triggered by the `SOLCOM` variable in the launch script. If `SOLCOM` is set to 1, the `-solcom` option is automatically added to the Kernel command line. The variable IFOENV in the FORTRAN code will be set to 0 if the `-solcom` option has been used, otherwise it will be set to 1.

- `-iasize n`: specifies the size `n` of the macro-array of integers IA (number of integers in the array). If the size is not sufficient, *Code_Saturne* stops and indicates the additional size needed.
  The value of `n` is to be placed in the `LONGIA` variable in the launch script. The option `-iasize $LONGIA` is automatically added to the Kernel command line.
  The value of `n` is accessible in the variable LONGIA in the FORTRAN code.

- `-rasize n`: specifies the size `n` of the macro-array of reals RA (number of reals in the array). If the size is not sufficient, *Code_Saturne* stops and indicates the additional size needed.
  The value of `n` is to be placed in the `LONGRA` variable in the launch script. The option `-rasize $LONGRA` is automatically added to the Kernel command line.
  The value of `n` is accessible in the variable LONGRA in the FORTRAN code.

- `-p n` or `-parallel n`: specifies the number of processors (potentially virtual) on which the Kernel will run. In the launch script, the number of processors used is specified in the `NOMBRE_DE_PROCESSEURS` variable, or through the batch headers. If necessary, the launch script then automatically passes the `-p` option to the Kernel command line (see 2.6).

- `--coupl-cs`: this option concerns the coupling of different executions of *Code_Saturne*. It is still under development. Please refer to *Code_Saturne* development team for further information.

- `-syrthes`: triggers the coupling with the code SYRTHES (thermal diffusion and transparent radiation in a solid). It has to be combined with a selection sub-option, to specify the boundary faces that need to be coupled. The syntax for selecting the faces is similar to that in the Preprocessor command line, with keywords `color` (for color selection), `group` (for group selection) and `invsel` (to invert the selection). See [9] for further details. For instance, to couple all the boundary faces except the faces of color 2 and 3, the command line option would be
  `-syrthes -color 2 3 -invsel`
  It is possible to couple a *Code_Saturne* calculation with a 2D SYRTHES calculation. To do so, the sub-option `-2d` must be added, potentially completed by the specification of the direction normal to the 2D mesh: `-X`, `-Y` or `-Z` (default). For instance:
  `-syrthes -group PAROI -2d -X`
  All these options are to be placed in the `COMMANDE_SYRTHES` variable of the launch script to be passed automatically to the Kernel command line.
  To be thourough, there are two other sub-options to the `-syrthes` option: `-proc n` the specify that the SYRTHES executable is running on the processor `n` and `-socket` in to specify that the communication between Code_Saturne and SYRTHES is made through sockets. These options are not to be specified by the user. They are automatically set and passed to the command line by the launch script.

- `-q n` or `--quality n`: triggers the verification mode. The code runs without any Interface parameter file nor any user subroutine. The mesh is read and elementary tests are performed.
  `n=-1`: no test (default value if no `-q` option is specified. The code runs normally
  `n=0`: the quality criteria of the mesh are calculated (non-orthogonality angles, internal faces off-set, ...) and corresponding EnSight post-processing parts are created.
  `n=1`: test calculation of the gradient of $sin(x + 2y + 3z)$. The calculated value is compared to the exact value, and an EnSight part for the corresponding error is created. The gradient is calculated with option IMRGRA=0.
  `n=2`: test calculation of the gradient of $sin(x + 2y + 3z)$. The calculated value is compared to the exact value, and an EnSight part for the corresponding error is created. The gradient is calculated with option IMRGRA=1.
  `n=3`: test calculation of the gradient of $sin(x + 2y + 3z)$. The calculated value is compared to the exact value, and an EnSight part for the corresponding error is created. The gradient is calculated with option IMRGRA=2.
  `n=4`: test calculation of the gradient of $sin(x + 2y + 3z)$. The calculated value is compared to the exact value, and an EnSight part for the corresponding error is created. The gradient is calculated with option IMRGRA=3.
  `n=5`: test calculation of the gradient of $sin(x + 2y + 3z)$. The calculated value is compared to the exact value, and an EnSight part for the corresponding error is created. The gradient is

calculated with option IMRGRA=4.
The command `-q n` is to be placed in the `ARG_CS_VERIF` variable in the launch script to be added automatically to the Kernel command line.
The value of `n` is accessible in the variable IVERIF in the FORTRAN code.

- `-cwf`: triggers the cutting of boundary and internal faces which have a warp angle larger than a certain limit[7]. The concerned faces are divided into triangles. This option is to handle with care, since the division of the faces increases the non-orthogonalities of the mesh, but it is sometimes required (for the Lagrangian modeling, for instance, where non-plane faces lead to noticeable particle loss). By default, the faces are divided if their warp angle is larger than 0.01 degrees. This default value can be changed by adding an optional angle value to the command. For instance, to devide faces with a warp angle larger than 0.02 degrees, the full option will be `-cwf 0.02`.
This option is to be specified in the `COMMANDE_DF` variable in the launch script, to be automatically passed to the command line.

- `--benchmark`: triggers the benchmark mode, for a timing of elementary operations on the machine. A secondary option `--mpitrace` can be added. It is to be activated when the benchmark mode is used in association with a MPI trace utility. It restricts the elementary operations to those implying MPI communications and does only one of each elementary operation, to avoid overfilling the MPI trace report.
This command is to be placed in the `ARG_CS_VERIF` variable in the launch script to be added automatically to the Kernel command line.

- `--log n`: specifies the destination of the output for a monoprocessor calculation or for the processor of rank 0 in a parallel calculation.
`n=0`: output directed towards the standard output
`n=1`: output redirected towards a file `listing` (default behaviour)
This option can be specified in the `ARG_CS_OUTPUT` variable of the launch script.

- `--logp n`: specifies the destination of the output for the processors of rank 1 to $N-1$ in a calculation in parallel on N processors (*i.e.* the redirection of all but the first processor).
`n=-1`: no output for the processors of rank 1 to $N-1$ (default behaviour).
`n=0`: no redirection. Every processor will write to the standard output. This might be useful in case a debugger is used, with separate terminals for each processor.
`n=1`: one file for the output of each processor. The output of the processors of rank 1 to $N-1$ are directed to the files `listing_n0002` to `listing_n`N. This option can be specified in the `ARG_CS_OUTPUT` variable of the launch script.

- `-param xxx`: specifies the name of the Interface parameter file to use for the calculation.
The value of `xxx` is to be placed in the `PARAM` variable in the launch script (the file will be looked for in the directory `DATA`). The option `-param $PARAM` is automatically added to the Kernel command line.

- `-h` or `--help`: to display a summary of the different command line options.

2.6 Parameters in the launch script

The case preparer `cree_sat` places an example of launch script, `lance`, in the `SCRIPTS` directory. This script is quite general and known to work on every architecture *Code_Saturne* has been tested on. The beginning if the script contains the definition of certain parameters (environment variables) necessary to set the calculation. The second part of the script contains the commands for the preparation and execution of the calculation. No user intervention should be necessary in this second part.
The Graphical User Interface allows to fill in the major parameters of the script without having to edit the file.

[7] the warp angle is an indicator of the non-coplanarity of the different vertices of the face

Below is a list of the different variables and parameters that might be modified for a calculation, in their order of apparition in the script:

- LSF headers: definition of the headers for an LSF batch system, as can be found on the machines of the CCRT (Tantale/Platine). The data expected are the number of processors reserved (`#BSUB -n`), the CPU time limit (`#BSUB -W`), the name of the standard output file (`#BSUB -o`), the name of the standard error file (`#BSUB -e`) and the name of the job (`#BSUB -J`).
- PBS headers: definition of the headers for a PBS batch system, as can be found on the machines of the Chatou cluster. The data expected are the number of nodes reserved (`nodes`), the number of processors per node (`ppn`), the total CPU time (`walltime`), the memory reserved (`mem`), and the name of the job (`#PBS -N`).
- Manchester headers: definition of the headers for the batch system specific to the cluster of the University of Manchester
- `SOLCOM`: a value of 1 will pass the `-solcom` option to the Kernel (see 2.5)
- `LONGIA`: value of the parameter LONGIA to be passed to the Kernel through the `-iasize` option (see 2.5).
- `LONGRA`: value of the parameter LONGIA to be passed to the Kernel through the `-rasize` option (see 2.5)

For parallel computations, LONGIA and LONGRA can theoretically be divided by the number of processors with respect to their value in a single-processor calculation, since each execution only deals with a fraction of the domain. It is however advised to add a safety margin (10%) to account for non-optimal distribution of the domain among the processors and for the presence of phantom cells (see §3.7).

- `ETUDE`: name of the study directory (automatically set by `cree_sat`, see §2.1.2)
- `CAS`: name of the case directory (automatically set by `cree_sat`, see §2.1.2)
- `PARAM`: name of the Interface parameter file, if necessary (see 2.5)
- `MAILLAGE`: name(s) of the mesh(es) used for the calculation (see 2.4.2 and 2.4.1). The files will be looked for in the directory `REPMAIL` (see below).
- `COMMANDE_RC`: Preprocessor command line option for mesh pasting (see 2.4.2)
- `COMMANDE_DF`: Kernel command line option for the division of faces with too large a warp angle (see 2.5)
- `COMMANDE_PERIO`: Preprocessor command line option for the definition of periodic boundary conditions (see 2.4.2)
- `COMMANDE_SYRTHES`: Kernel command line option for coupling with SYRTHES (see 2.5)
- `DONNEES_THERMOCHIMIE`: name of the thermochemical data file, if necessary (the file is looked for in the directory `DATA`, see §4.31)
- `NOMBRE_DE_PROCESSEURS`: number of processors (potentially virtual) to be used for the calculation.
  If the variable is left empty, the launch script will fill it automatically: on a batch system, `NOMBRE_DE_PROCESSEURS` will be equal to the number of processors reserved; in case of an interactive calculation, it will be set to 1.
  When using a batch system, `NOMBRE_DE_PROCESSEURS` should ideally be equal to the number of processors reserved, and can never be larger (one executable per processor). With an interactive

calculation (like a Linux PC), NOMBRE_DE_PROCESSEURS can be larger than the total number of processors available, although it is not recommended (loss of efficiency because several executables share the same processor).
In case of coupling with SYRTHES, one processor is reserved for SYRTHES, and the Kernel of *Code_Saturne* will therefore automatically be set to run on NOMBRE_DE_PROCESSEURS-1 processors.

- LISTE_PROCESSEURS: list of nodes on which the calculation is to be run. On batch systems, this list is set automatically by the batch manager. For calculations on a stand-alone machine, the list is not used. Hence, except for very specific test (mainly for developing purposes), it is recommended to leave this variable empty.

- FICHIERS_DONNEES_UTILISATEUR: list of the user data files to be copied in the temporary execution directory before the calculation (input profiles for instance). The files will be looked for in the directory DATA. The thermochemical data files, Interface parameter file and calculation restart files are specified in other variables and do not need to appear here. When using the vortex method for LES entry conditions, the corresponding data files have to be specified in FICHIERS_DONNEES_UTILISATEUR (see §4.5)

- FICHIERS_RESULTATS_UTILISATEUR: list of user result files to be copied in the directory RESU at the end of the calculation. A directory RES_USERS.mmddhhmm will be created in the directory RESU and all the files will be stored in it. The files automatically created by the code (listings, post-processing, automatic chronological records[8], restart files) do not need to be specified in FICHIERS_RESULTATS_UTILISATEUR.

- CS_TMP_PREFIX: alternate temporary directory for the calculation (see §2.2.2)

- OPTIMISATION: optimisation level for compilation (LO, DBG, EF, PROF or PUR; see §2.1.3). This optimisation level will be applied to all the modules of *Code_Saturne* (BASE, CFBL, COGZ, CPLV, ELEC, FUEL, LAGR, MATI, RAYT). Leaving the variable empty stands for "standard" optimisation.

- LISTE_LIB_SAT: list of *Code_Saturne* module libraries to use (see §2.1.3). Specifying a list allows to use different optimisation options for different modules. If a list is given, all modules must be referenced once (and only once). Leaving the variable empty implies taking the same optimisation for all the modules (BASE, COGZ, CFBL, CPLV, ELEC, FUEL, LAGR, MATI, RAYT), corresponding to the value of the OPTIMISATION variable (see above). An example of list could be:
```
LISTE_LIB_SAT=''libsaturneBASEDBG.a libsaturneCFBL.a libsaturneCOGZDBG.a \
               libsaturneCPLV.a libsaturneELECDBG.a libsaturneFUELDBG.a \
               libsaturneLAGR.a libsaturneMATI.a libsaturneRAYT.a''
```

- OPTION_LIB_EXT: additional commands for the link stage of the compilation. This can be especially useful if the user subroutines call routines provided by external libraries. To link with an external library "foo", the variable would be for instance
```
OPTION_LIB_EXT=''-L/opt/foo/lib -lfoo''
```

- VALGRIND: command to be placed before the *Code_Saturne* executable name on the execution command line (*i.e.* the launch script will execute the command `$VALGRIND cs13.exe ...`). It is especially designed to use the valgrind debugging and profiling tool. The usual value to use valgrind is `VALGRIND=''valgrind --tool=memcheck''`

- ARG_CS_VERIF: verification mode to be used for *Code_Saturne* (see 2.5). An empty variable implies standard calculation mode (IVERIF=-1).

- ARG_CS_OUTPUT: options for the redirection of the standard output (see 2.5)

- ECHOCOMM: level for the `--echo-comm` option of the Kernel command line (see 2.5)

[8] when using `ushist` for user-defined chronological records, the files created need to be specified in FICHIERS_RESULTATS_UTILISATEUR

- `PILOTAGE_ADAPTATION`: commands to trigger the automatic mesh adaptation with the software Homard. This option is still under development and restricted to developpers use.
- `REPBASE`: root directory of the calculation. This variable is automatically set by `cree_sat` and should not be changed.
- `DATA`: DATA directory of the case (see 2.1.2). This variable is automatically set by `cree_sat` and should not be changed.
- `RESU`: RESU directory of the case (see 2.1.2). This variable is automatically set by `cree_sat` and should not be changed.
- `FORT`: FORT directory of the case (see 2.1.2). This variable is automatically set by `cree_sat` and should not be changed.
- `SCRIPTS`: SCRIPTS directory of the case (see 2.1.2). This variable is automatically set by `cree_sat` and should not be changed.
- `SUITE_AMONT`: directory containing the files for calculation restart.
- `PRE_TRAITEMENT_AMONT`: directory containing the `enveloppe_vers_solveur*` files for a calculation in "calculation" mode (see 2.2.3)
- `REPMAIL`: directory containing the mesh files (see 2.1.2). This variable is automatically set by `cree_sat` and should generally not be changed.
- `DATA_SYR`: directory for the SYRTHES data. This directory has to be created by the user. It is advised to keep the location proposed in the launch script, which complies with the standard architecture of *Code_Saturne* (see 2.1.2).
- `SYRTHES_ENV`: name of the environment file for SYRTHES (usually `syrthes.env`, as proposed in the launch script).
- `FORT_SYR`: directory for the SYRTHES user subroutines. This directory has to be created by the user. It is advised to keep the location proposed in the launch script, which complies with the standard architecture of *Code_Saturne* (see 2.1.2).
- `MODE_COUPLAGE`: coupling mode between *Code_Saturne* and SYRTHES, when such coupling is activated (see `COMMANDE_SYRTHES`). Three options are available:
  `MPI`: for a coupling based on MPI messages (requires an MPI library)
  `pipes`: for a coupling based on pipe files (on clusters, such a coupling is valid only if all the processors are located on the same node)
  `sockets`: for a coupling based on sockets
- `MODE_EXEC`: execution mode for *Code_Saturne* (see 2.2.3)

2.7 Graphical User Interface

A Graphical User Interface is available with *Code_Saturne*. This Interface creates or reads an XML file according to a specific *Code_Saturne* syntax which is then interpretated by the code.

In version 1.3.2, the Graphical Interface manages calculation parameters, standard initialisation values and boundary conditions for standard physics, pulverised coal combustion and radiative transfers. The other specific physics are not yet managed by the Graphical Interface. In these particular cases, user subroutines have to be completed.

The Interface is optionnal. Every data that can be specified through the Interface can also still be specified in the user subroutines. In case of conflict, all calculation parameters, initialisation value or boundary condition set directly in the user subroutines will prevail over what is defined by the

Interface. However, it is no longer necessary to redefine everything in the user subroutines. Only what was not set or could not be set using the Graphical Interface should be specified.

WARNING: There are some limitations to the changes that can be made between the Interface and the user routines. In particular, it is not possible to specify a certain number of solved variables in the Interface and change it in the user routines (for example, it is not possible to specify the use of a $k-\varepsilon$ model in the Interface and change it to $R_{ij}-\varepsilon$ in `usini1.F`, or to define additional scalars in `usini1` with respect to the Interface). Also, all boundaries should be referenced in the Interface, even if the associated conditions are intended to be modified in `usclim`, and their nature (entry, outlet, wall[9], symmetry) should not be changed.

For example, in order to set the boundary conditions of a calculation corresponding to a channel flow with a given inlet velocity profile, one should:
- set the boundary conditions corresponding to the wall and the output using the Graphical Interface - set a dummy boundary condition for the inlet (uniform velocity for instance) - set the proper velocity profile at inlet in `usclim`. The wall and output areas do not need to appear in `usclim`. The dummy velocity entered in the Interface will not be taken into account.

The Graphical User Interface is launched with the `./SaturneGUI` command in the directory `DATA`. The first step is then to load an existing parameter file (in order to modify it) or to open a new one. The headings to be filled for a standard calculation are the followings:

- Analysis environment: definition of the calculation directories (STUDY, CASE), mesh file(s), periodicity, coupling with SYRTHES, stand-alone execution of the Preprocessor module (used by the Interface to get the colors of the boundary faces).

- Thermophysical models: physical model, ALE mobile mesh features, turbulence model, thermal model, initialisation of the variables.

- Physical properties: reference pressure, fluid characteristics, gravity.

- Additional scalars: definition, physical characteristics and initialisation of the scalars (apart from the temperature, which is treated separately in the Interface).

- Boundary conditions: definition of the boundary conditions for each variable. The colors of the boundary faces may be read directly from a "listing" file created by the Preprocessor. This file can be generated directly by the Interface under the heading
"Analysis environment → Solution Domain → Stand-alone running".

- Analysis control: parameters concerning the time averages, time step, location of the probes where some variables will be monitored over time, definition of the periodicity of the outputs in the calculation listing and in the chronological records and of the EnSight outputs.

- Numerical parameters: advanced parameters for the numerical solution of the equations

- Calculation management: management of the calculation restarts, updating of the launch script (temporary execution directory, parallel computing, user data or result files, ...), interactive launch of the calculation and user arrays definition.

The *Code_Saturne* tutorial [14] offers a step-by-step guidance to the setting up of some simple calculations with the *Code_Saturne* Interface.

To launch *Code_Saturne* using an XML parameter file, the name of the file must be given to the variable `PARAM` in the launch script (see §2.6). When the launch script is edited from the Interface (Calculation management → Prepare batch analysis), the PARAM section is filled automatically as are the other parameters specified through the Interface.

[9] smooth and rough walls are considered of the same nature

NOTE: OPTION `-noihm` OF CREE_SAT
When a calculation is using the Interface but, for some reason, some extra parameters need to be specified in the subroutine `usini1`, the latter must be placed in the directory `FORT`. But, while doing this, all the parameters appearing in `usini1` will also be taken into account. In order to prevent the user from having to respecify in `usini1` all that he has already specified through the Interface, `cree_sat` automatically comments out the examples in `usini1` (`Cex` at the beginning of each line) while copying it in the directory `USERS`. Therefore, the user only needs to uncomment the specific parts of `usini1` he wants to modify, and the rest of the examples will be ignored.
On the contrary, if the Interface will not be used, then all the parameters in `usini1` have to be specified. In that case, using the `-noihm` option of `cree_sat` will prevent it from commenting `usini1` out, thus saving the user the tedious task of uncommenting all the lines (and the risk of skipping some of them).

2.8 Face and cell mesh-defined properties and selection

The mesh entities may be referenced by the user during the mesh creation. These references may then be used to mark out some mesh entities according to the need (specification of boundary conditions, pressure drop zones ...). The references are generally of one of the two following types:

- color. A color is an integer possibly associated with boundary faces and volume elements by the mesh generator. Depending on the tool, this concept may have different names, which *Code_Saturne* interprets as colors. Most tools allow only one color per face or element.
  - I-deas uses a color number with a default of 7 (green) for elements, be they volume elements or boundary "surface coating" elements. Color 11 (red) is used for for vertices, but vertex properties are ignored by *Code_Saturne*.
  - SIMAIL uses the equivalent notions of "reference" for element faces, and "subdomain" for volume elements. By default, element faces are assigned no reference (0), and volume elements domain 1.
  - Gmsh uses "physical property" numbers.
  - EnSight has no similar notion, but if several parts are present in an EnSight 6 file, or several parts are present *and* vertex ids are given in an Ensight Gold file, the part number is interpreted as a color number by the Preprocessor.
  - The Comet Design (pro-STAR/STAR4) and NUMECA Hex file formats have an CAD section id that is interpreted as a color number. In the latter case, this notion only applies to faces, so volume elements are given color.
  - The MED format allow integer "attributes", though many tools working with this format ignore those and only handle groups.
- groups. Named "groups" of mesh entities may also be used with many mesh generators or formats. In some cases, a given cell or face may belong to multiple groups (as some tools allow new groups to be defined by boolean operations on existing groups). In *Code_Saturne*, every group is assigned a group number (base on alphabetical ordering of groups).
  - I-deas Master Series assigns a group number with each group, but by default, this number is just a counter. Only the group name is considered by *Code_Saturne* (so that elements belonging to two groups with identical names and different numbers are considered as belonging to the same group).
  - CGNS allows both for named boundary conditions and mesh sections. If present, boundary condition names are interpreted as group names, and groups may also be defined based on element section or zone names using additional Preprocessor options (`-grp-cel` or `-grp-fac` followed by `section` or `zone`).
  - Using the MED format, it is preferable to use "groups" to colors, as many tools ignore the latter.

Selection criteria may be defined in a similar fashion whether using the GUI or in user subroutines. Typically, a selection criteria is simply a string containing the required color numbers or group names, possibly combined using boolean expressions. Simple geometric criteria are also possible.

A few examples are given below:

```
ENTRY
1 or 7
all[]
3.1 >= z >= -2 or not (15 or entry)
range[04, 13, attribute]
sphere[0, 0, 0, 2] and (not no_group[])
```

Strings such as group names containing whitespace or having names similar to reserved operators may be protected using "escape characters".[10] More complex examples of strings whith protected strings are given here:

```
"First entry" or Wall\ or\ sym
entry or \plane or "noone's output"
```

The following operators and syntaxes are allowed (fully capitalized versions of keywords are also allowed, but mixed capitals/lowercase versions are not):

escape characters

protect next character only:	\
protect string:	*'string'* *"string"*

basic operators

priority:	( )
not:	not ! !=
and:	and & &&
or:	or | || , ;
xor:	xor ^

general functions

select all:	all[]
entities having no group or color:	no_group[]
select a range of groups or colors:	range[*first*, *last*]
	range[*first*, *last*, group]
	range[*first*, *last*, attribute]

For the range operator, *first* and *last* values are inclusive. For attribute (color) numbers, natural integer value ordering is used, while for group names, alphabetical ordering is used. Note also that in the bizarre (not recommended) case in which a mesh would contain for example both a color number 15 and a group named "15", using `range[15, 15, group]` or `range[15, 15, attribute]` could be used to distinguish the two.

Geometric functions are also available. The coordinates considered are those of the cell or face centers. Normals are of course usable only for face selections, not cell selections.

[10] Note that for defining a string in Fortran, double quotes are easier to use, as they do not conflict with Fortran's single quotes delimiting a string. In C, the converse is true. Also, in C, to define a string such as `\plane`, the string `\\plane` must be used, as the first \ character is used by the compiler itself. Using the GUI, either notation is easy.

geometric functions

face normals:	`normal[`x`, `y`, `z`, `*epsilon*`]` `normal[`x`, `y`, `z`, epsilon = `*epsilon*`]`

plane, $ax + by + cz + d = 0$ form:	`plane[`a`, `b`, `c`, `d`, `*epsilon*`]`
	`plane[`a`, `b`, `c`, `d`, epsilon = `*epsilon*`]`
	`plane[`a`, `b`, `c`, `d`, inside]`
	`plane[`a`, `b`, `c`, `d`, outside]`

plane, normal + point in plane form:	`plane[`n_x`, `n_y`, `n_z`, `x`, `y`, `z`, `*epsilon*`]`
	`plane[`n_x`, `n_y`, `n_z`, `x`, `y`, `z`, epsilon = `*epsilon*`]`
	`plane[`n_x`, `n_y`, `n_z`, `x`, `y`, `z`, inside]`
	`plane[`n_x`, `n_y`, `n_z`, `x`, `y`, `z`, outside]`

box, extents form:	`box[`x_{min}`, `y_{min}`, `z_{min}`, `x_{max}`, `y_{max}`, `z_{max}`]`

box, origin + axes form:	`box[`x_0`, `y_0`, `z_0`,`
	`  `dx_1`, `dy_1`, `dz_1`, `dx_2`, `dy_2`, `dz_2`, `dx_3`, `dy_3`, `dz_3`]`
	`plane[`a`, `b`, `c`, `d`, epsilon = `*epsilon*`]`
	`plane[`a`, `b`, `c`, `d`, inside]`
	`plane[`a`, `b`, `c`, `d`, outside]`

cylinder:	`cylinder[`x_0`, `y_0`, `z_0`, `x_1`, `y_1`, `z_1`, `*radius*`]`
sphere:	`sphere[`x_c`, `y_c`, `z_c`, `*radius*`]`
inequalities:	`>`, `<`, `>=`, `<=` associated with `x`, `y`, `z` or `X`, `Y`, `Z` keywords and coordinate value; x_{min} `<= x <` x_{max} type syntax is allowed.

In the current version of *Code_Saturne*, all selection criteria used are maintained in a list, so that re-interpreting a criterion already encountered (such as at the previous time step) is avoided. Lists of entities corresponding to a criteria containing no geometric functions are also saved in a compact manner, so re-using a previously used selection should be very fast. For criteria containing geometric functions, the full list of corresponding entities is not maintained, so each entity must be compared to the criterion at each time step. Heavy use of many selection criteria containing geometric functions may thus lead to reduced performance.

3 Main variables

This section presents a non-exhaustive list of the main variables which may be encountered by the user. Most of them should not be modified by the user. They are calculated automatically from the data. However it may be useful to know what they represent. Developpers can also refer to [3] and [11].

These variables are listed in the alphabetical index at the end of this document.

The type of each variable is given: integer [I], real number [R], integer array [IA], real array [RA].

3.1 Array sizes

NDIM [I] : Space dimension (NDIM=3).

NCEL [I] : Number of real cells in the mesh.

NCELET [I] : Number of cells in the mesh, including the ghost cells of the "halos" (see note 1).

NFAC [I] : Number of internal faces (see note 2).

NFABOR [I] : Number of boundary faces (see note 2).

NCELBR [I] : Number of cells with at least one boundary face (see note 2).

LNDFAC [I] : Size of the array NODFAC of internal faces - nodes connectivity (see note 3).

LNDFBR [I] : Size of the array NODFBR of boundary faces - nodes connectivity (see note 3).

NNOD [I] : Number of vertices in the mesh.

NFML [I] : Number of referenced families of entities (boundary faces, elements, ...).

NPRFML [I] : Number of properties per referenced entity family.

NPHAS [I] : Effective number of phases. NPHAS must be inferior or equal to NPHSMX. In the current version, NPHAS is forced to 1 and should not be changed..

NPHSMX [I] : Maximum number of phases (default value: 1)[11].

NVAR [I] : Number of solved variables (must be lower than NVRMAX).

NSCAMX [I] : Maximum number of scalars solutions of an advection equation, apart from the variables of the turbulence model (k, ε, R_{ij}, ω, φ, $\overline{f}$). That is to say the temperature and other scalars (passive or not, user-defined or not).

NSCAL [I] : Effective number of scalars solutions of an advection equation, apart from the variables of the turbulence model (k, ε, R_{ij}, ω, φ, $\overline{f}$). That is to say the temperature and other scalars (passive or not, user-defined or not). These scalars can be divided into two distinct groups: NSCAUS user-defined scalars and NSCAPP scalars related to a "specific physics". NSCAL=NSCAUS+NSCAPP, and NSCAL must be inferior or equal to NSCAMX.

NSCAPP [I] : Effective number of scalars related to a "specific physics". These scalars are solutions of an advection equation and distinct from the scalars of the turbulence model (k, ε, R_{ij}, ω, φ, $\overline{f}$). They are automatically defined by the choice of the selected specific physics model (gas combustion with Eddy Break-Up model, pulverised coal combustion, ...). For example: mass fractions, enthalpy, ...

NSCAUS [I] : Effective number of user-defined scalars. These scalars are solutions of an advection equation and distinct from the scalars of the turbulence model (k, ε, R_{ij}, ω, φ, $\overline{f}$) and from the NSCAPP scalars related to the "specific physics". For example: passive tracers, temperature (when no specific physics model is selected), ...

NESTMX [I] : Maximum number of error estimators for Navier-Stokes.

LONGIA [I] : Size of the macro array of integer IA.

LONGRA [I] : Size of the macro array of real RA.

NPROMX [I] : Maximum number of physical properties. They will be stored in the arrays PROPCE, PROPFA or PROPFB.

NPROCE [I] : Number of properties defined at the cells. They will be stored in the array PROPCE.

NPROFA [I] : Number of properties defined at the internal faces. They will be stored in the array PROPFA.

NPROFB [I] : Number of properties defined at the boundary faces. They will be stored in the array PROPFB.

NVISLS [I] : Number of scalars with variable diffusivity.

NUSHMX [I] : Maximum number of user chronological files (in the case where `ushist` is used).

NBMOMT [I] : Effective number of calculated time-averages. NBMOMT must be inferior or equal to NBMOMX.

[11] the data structure of *Code_Saturne* is ready for a multiphase description, however no multiphase model has been implemented. Moreover, some options of the code are not compatible with NPHAS different from 1.

NBMOMX [I] : Maximum number of calculated time-averages (default value: 50).

NDGMOX [I] : Maximum degree of the time-averages (default value: 5).

NCLACP [I] : Number of coal classes for the pulverised coal combustion module. It is the total number of classes, *i.e.* the sum of the number of classes for every represented coal. NCLACP must be inferior or equal to NCLCPM.

NCLCPM [I] : Maximum number of coal classes for the pulverised coal combustion module.

Note 1: ghost cells - "halos"

A cell (real cell) is an elementary mesh element of the spatial discretisation of the calculation domain. The mesh is made of NCEL cells.

When using periodicity and parallelism, extra "ghost" cells (called "halo" cells) are defined for temporary storage of some information (on a given processor). The total number of real and ghost cells is NCELET.

Indeed, when periodicity is enabled, the cells with periodic faces do not have any real neighboring cell across these particular faces. Their neighboring cell is elsewhere in the calculation domain (its position is determined by the periodicity). In order to temporarily store the information coming from this "distant" neighboring cell, a ghost cell ("halo") is created.

The same kind of problem exists in the case of a calculation on parallel machines: due to the decomposition of the calculation domain, some cells no longer have access to all their neighboring cells, some of them being treated by another processor. The creation of ghost cells allows to temporarily store the information coming from real neighboring cells treated by other processors.

The variables are generally arrays of size NCELET (number of real and fictitious cells). The calculations (loops) are made on NCEL cells (only the real cells, the fictitious cells are only used to store information).

Note 2: internal faces

An internal face is an inferface shared by two cells (real or ghost ones) of the mesh. A boundary face is a face which has only one real neighboring cell. In the case of periodic calculations, a periodic face is an internal face. In the case of parallel running calculations, the faces situated at the boundary of a partition may be internal faces or boundary faces (of the whole mesh);

Note 3: faces-nodes connectivity

The faces - nodes connectivity is stored by means of four integer arrays: IPNFAC and NODFAC for the internal faces, IPNFBR and NODFBR for the boundary faces. NODFAC (dimension LNDFAC) contains the list of all the nodes of all the internal faces; first the nodes of the first face, then the nodes of the second face, and so on. IPNFAC (dimension: NFAC+1) gives the position IPNFAC(IFAC) in NODFAC of the first node of each internal face IFAC. Therefore, the reference numbers of all the nodes of the internal face IFAC are : NODFAC(IPNFAC(IFAC)), NODFAC(IPNFAC(IFAC)+1), ..., NODFAC(IPNFAC(IFAC+1)-1). In order for this last formula to be valid even for IFAC=NFAC, IPNFAC is of dimension NFAC+1 and IPNFAC(NFAC+1) is equal to LNDFAC+1.

The composition of the arrays NODFBR and IPNFBR is similar.

Note 4: commons

The user will not modify the existing "commons". This would require the recompilation of the complete version, operation which is not allowed in standard use.

3.2 Geometric variables

The main geometric variables are available in most of the subroutines and directly accessible through the following arrays.

CDGFAC(NDIM,NFAC) [RA] : Coordinates of the centers of the internal faces.

CDGFBO(NDIM,NFABOR) [RA] : Coordinates of the centers of the boundary face.

IFACEL(2,NFAC) [IA] : Index-numbers of the two (only) neighboring cells for each internal face.

IFABOR(NFABOR) [IA] : Index-number of the (unique) neighboring cell for each boundary face.

IPNFAC(NFAC+1) [IA] : Position of the first node of the each internal face in the array NODFAC (see note 3 in paragraph 3.1)..

IPNFBR(NFABOR+1) [IA] : Position of the first node of the each boundary face in the array NODFBR (see note 3 in paragraph 3.1)..

NODFAC(LNDFAC) [IA] : Index-numbers of the nodes of each internal face (see note 3 in paragraph 3.1)..

NODFBR(LNDFBR) [IA] : Index-numbers of the nodes of each boundary face (see note 3 in paragraph 3.1)..

SURFAC(NDIM,NFAC) [RA] : Surface vector of the internal faces. Its norm is the surface of the face and it is oriented from IFACEL(1,.) to IFACEL(2,.)..

SURFBO(NDIM,NFABOR) [RA] : Surface vector of the boundary faces. Its norm is the surface of the face and it is oriented outwards.

VOLUME(NCELET) [RA] : Volume of each cell.

XYZCEN(NDIM,NCELET) [RA] : Coordinates of the cell centers.

XYZNOD(NDIM,NNOD) [RA] : Coordinates of the mesh vertices.

In addition, other geometric variables are accessible in sections of the unidimensional macro-arrays IA (for integers) and RA (for real numbers) which are passed as arguments in every subroutine (apart from a few ones of very low level). The index-number of the first element of these sections is stored in a "common" (in the file `pointe.h`), passed to most of the routines. Hence, the surface of an internal face IFAC is stored in RA(ISRFAN+IFAC-1). Or, the coordinate of vector $\underline{OF}$ (see below for definition) in the II^{th} direction for face IFAC is stored in RA(IDOFIJ+(IFAC-1)*NDIM+II-1)[12].

The main variables of this type are the following:

IDIJPF [I] : In RA, pointer to DIJPF(NDIM,NFAC), real array giving, for every internal face, the three components of the vector $\underline{I'J'}$, where I' and J' are respectively the orthogonal projections of the neighboring cell centers I and J on a straight line orthogonal to the face and passing through its center..

IDIIPB [I] : In RA, pointer to DIIPB(NDIM,NFABOR), real array giving, for every boundary face, the three components of the vector $\underline{II'}$. I' is the orthogonal projection of I, center of the neighboring cell, on the straight line perpendicular to the face and passign through its center.

IDIST [I] : In RA, pointer to DIST(NFAC), real array giving, for every internal face, the scalar product between the vectors $\underline{IJ}$ and $\underline{n}$. I and J are respectively the centers of the first and the second neighboring cell. The vector $\underline{n}$ is the unit vector normal to the face and oriented from the first to the second cell.

IDISTB [I] : In RA, pointer to DISTBR(NFABOR), real array giving, for every boundary face, the scalar product between the vectors $\underline{IF}$ and $\underline{n}$. I is the center of the neighboring cell. F is the face center. The vector $\underline{n}$ is the unit vector normal to the face and oriented to the exterior of the domain.

IDOFIJ [I] : In RA, pointer to DOFIJ(NDIM,NFAC), real array giving, for every internal face, the

[12] in FORTRAN, a multidimensional array A(3,2) is in fact a unidimensional array containing the elements A(1,1), A(2,1), A(3,1), A(1,2), A(2,2) and A(3,2) in this order.

components of the vector $\underline{OF}$. O is the intersection point between the face and the straight line joining the centers of the two neighboring cells. F is the face center.

IICELB [I] : In IA, pointer to ICELBR(NCELBR), integer array giving the list of cells havong at least one boundary face.

IPOND [I] : In RA, pointer to POND(NFAC), real array giving $\frac{\underline{FJ}.\underline{n}}{\underline{IJ}.\underline{n}}$, for every internal face. With regard to the mesh quality, its ideal value is 0.5.

ISRFAN [I] : In RA, pointer to SURFAN(NFAC), real array giving the norm of the surface vector of the internal faces.

ISRFBN [I] : In RA, pointer to SURFBN(NFABOR), real array giving the norm of the surface of the boundary faces.

3.3 Physical variables

The main physical variables are available in the majority of the subroutines and brought together according to their type in the multidimensional arrays listed below. In some paricular subroutines, some variables may be given a more explicit name, in order to ease the comprehension.

PROPCE(NCELET,NPROCE) [RA] : Properties defined at the cell centers. For instance: density, viscosity ....

PROPFA(NFAC,NPROFA) [RA] : Properties defined at the internal faces. For instance: mass flow across internal faces.

PROPFB(NFABOR,NPROFB) [RA] : Properties defined at the boundary faces. For instance: mass flow across boundary faces, density at boundary faces ....

RTP(NCELET,NVAR) [RA] : Array storing the values of the solved variables at the current time step.

RTPA(NCELET,NVAR) [RA] : Array storing the values of the solved variables at the previous time step.

Concerning RTP and RTPA

The indexes allowing to mark out the different variables (from 1 to NVAR) are integers available in a "common" file called `numvar.h`. Some solved variables (pressure, velocity, turbulence) depend on the considered phase, and the index which refers to it is then a array of size NPHSMX, the maximum number of phases.

For example, IPR(IPHAS) refers to the variable "pressure" of the phase IPHAS (with $1 \leqslant$IPHAS$\leqslant$NPHAS): the pressure of the phase IPHAS in the cell IEL at the current time step is therefore RTP(IEL,IPR(IPHAS)).

The list of integers referring to solved variables is given below. These variable index-numbers are not only used for the RTP and RTPA arrays, but also for some arrays of variable associated options (for instance, BLENCV(IK(IPHAS)) is the percentage of second-order convective scheme for the turbulent energy of the phase IPHAS when a corresponding turbulent model is used).

- IPR(IPHAS): pressure[13].
- IU(IPHAS): velocity along the X axis.
- IV(IPHAS): velocity along the Y axis.
- IW(IPHAS): velocity along the Z axis.

[13] IPR(IPHAS) corresponds to a reduced pressure, from which the standard hydrostatic pressure has be deduced. The total pressure is stored in the PROPCE array

- IK(IPHAS): turbulent energy, in $k-\varepsilon$, $k-\omega$ modeling or v2f (φ-model) modeling.
- IR11(IPHAS): Reynolds stress R11, in $R_{ij}-\varepsilon$ or SSG modeling.
- IR22(IPHAS): Reynolds stress R22, in $R_{ij}-\varepsilon$ or SSG modeling.
- IR33(IPHAS): Reynolds stress R33, in $R_{ij}-\varepsilon$ modeling.
- IR12(IPHAS): Reynolds stress R12, in $R_{ij}-\varepsilon$ modeling.
- IR13(IPHAS): Reynolds stress R13, in $R_{ij}-\varepsilon$ modeling.
- IR23(IPHAS): Reynolds stress R23, in $R_{ij}-\varepsilon$ modeling.
- IEP(IPHAS): turbulent dissipation in $k-\varepsilon$, $R_{ij}-\varepsilon$ or v2f (φ-model) modeling.
- IOMG(IPHAS): Specific dissipation rate ω, in $k-\omega$ SST modeling.
- IPHI(IPHAS): variable $\varphi=\overline{v^2}/k$ in v2f (φ-model).
- IFB(IPHAS): variable $\overline{f}$ in v2f (φ-model).
- ISCA(J): scalar J ($1\leqslant$J$\leqslant$NSCAL).

Concerning the solved scalar variables (apart from the variables pressure, k, ε, R_{ij}, ω, φ, $\overline{f}$), the following are highly important:

- The designation "scalar" refers to scalar variables which are solution of an advection equation, apart from the variables of the turbulence model (k, ε, R_{ij}, ω, φ, $\overline{f}$): for instance the temperature, scalars which may be passive or not, "user" or not. The mean value of the square of the fluctuations of a "scalar" is a "scalar", too. The scalars may be divided into two groups: NSCAUS "user" scalars and NSCAPP "specific physics" scalars, with NSCAL=NSCAUS+NSCAPP. NSCAL must be inferior or equal to NSCAMX.
- The phase related to the scalar J is IPHSCA(J).
- The J$^{\text{th}}$ user scalar is, in the whole list of the NSCAL scalars, the scalar number J. In the list of the NVAR solved variables, it corresponds to the variable number ISCA(J), its value in the cell IEL at the current time step is given by RTP(IEL,ISCA(J)).
- The J$^{\text{th}}$ scalar related to a specific physics is, in the whole list of the NSCAL scalars, the scalar number ISCAPP(J). In the list of the NVAR solved variables, it corresponds to the variable number ISCA(ISCAPP(J)), its value in the cell IEL at the current time step is given by RTP(IEL,ISCA(ISCAPP(J))).
- The temperature (or the enthalpy) is the scalar number ISCALT(IPHAS) in the list of the NSCAL scalars. It corresponds to the variable number ISCA(ISCALT(IPHAS)) and its value in the cell IEL is RTP(IEL,ISCA(ISCALT(IPHAS))). If there is no thermal scalar, ISCALT(IPHAS) is equal to -1.
- A "user" scalar number J may represent the average of the square of the fluctuations of a scalar K (*i.e.* the average $\overline{\varphi'\varphi'}$ for a fluctuating scalar φ). This can be made either *via* the interface or by indicating ISCAVR(J)=K in `usini1` (if the scalar in question is not a "user" scalar, the selection is made automatically). For instance, if J and K are "user" scalars, the variable φ corresponding to K is the variable number ISCA(K)=ISCA(ISCAVR(J)), and its value in the cell IEL is
  RTP(IEL,ISCA(K))=RTP(IEL,ISCA(ISCAVR(J))).
  The variable corresponding to the mean value of the square of the fluctuations[14] is the variable number ISCA(J) and its value in the cell IEL is RTP(IEL,ISCA(J)).

[14] it is really $\overline{\varphi'\varphi'}$, and not $\sqrt{\overline{\varphi'\varphi'}}$

Concerning PROPCE, PROPFA and PROPFB In *Code_Saturne*, the physical properties[15] are stored in the arrays PROPCE, PROPFA and PROPFB. Some properties, like the density, are only stored for cells and boundary faces. Some, like the mass flux, are only stored at the internal and boundary faces. To avoid having different index numbers for a physical property, depending on the array it is used in, the following structure is used in *Code_Saturne*:

- All the properties (used or not) have a unique and distinct index-number, given automatically by the code and stored in an integer or an integer array (its size may be the maximum number of phases, the maximum number of scalars or the maximum number of variables).

- The indexes referring to the different properties stored in the PROPxx arrays are given respectively by the following integer arrays:

  IPPROC(NPROMX) [IA] : Rank I in PROPCE(.,I) of the properties defined at the cell centers.

  IPPROF(NPROMX) [IA] : Rank I in PROPFA(.,I) of the properties defined at the internal faces.

  IPPROB(NPROMX) [IA] : Rank I in PROPFB(.,I) of the properties defined at the boundary faces.

For instance, the index number corresponding to the density of the phase IPHAS is IROM(IPHAS). In the list of the properties defined at the cell center, the density of the phase IPHAS is therefore the IPPROC(IROM(IPHAS))$^{\text{th}}$ property: its value at the center of the cell IEL is given by PROP**CE**(IEL,IPPRO**C**(IROM(IPHAS)))
In the same way, in the list of the properties defined at the boundary faces, the density of the phase IPHAS is the IPPROB(IROM(IPHAS)))$^{\text{th}}$ property: its value at the boundary face is given by PROP**FB**(IEL,IPPRO**B**(IROM(IPHAS)))

The list of properties accessible in the PROPxx arrays is given below (this does not include the properties linked to the specific physics modules):

IROM(NPHSMX) [IA] : For each phase, property number corresponding to the density (*i.e.* ρ in $kg.m^{-3}$)
stored at the cells and the boundary faces.

IROMA(NPHSMX) [IA] : For each phase, property number corresponding to the density (*i.e.* ρ in $kg.m^{-3}$) at the previous time step, in the case of a second-order extrapolation in time
stored at the cells and the boundary faces.

IVISCL(NPHSMX) [IA] : For each phase, property number corresponding to the fluid molecular dynamic viscosity (*i.e.* μ in $kg.m^{-1}.s^{-1}$)
stored at the cells.

IVISLA(NPHSMX) [IA] : For each phase, property number corresponding to the fluid molecular dynamic viscosity (*i.e.* μ in $kg.m^{-1}.s^{-1}$) at the previous time step, in the case of a second-order extrapolation in time
stored at the cells.

IVISCT(NPHSMX) [IA] : For each phase, property number corresponding to the fluid turbulent dynamic viscosity (*i.e.* μ_t in $kg.m^{-1}.s^{-1}$)
stored at the cells.

IVISTA(NPHSMX) [IA] : For each phase, property number corresponding to the fluid turbulent dynamic viscosity (*i.e.* μ_t in $kg.m^{-1}.s^{-1}$) at the previous time step, in the case of a second-order extrapolation in time
stored at the cells.

[15] other variables are stored in the arrays PROPCE, PROPFA and PROPFB. They are not "physical properties" strictly speaking, but it is convenient to have them in the same array as the proper physical properties

ICP(NPHSMX) [IA] : For each phase, property number corresponding to the specific heat, in case where it is variable (*i.e.* C_p in $m^2.s^{-2}.K^{-1}$). See note below
stored at the cells.

ICPA(NPHSMX) [IA] : For each phase, property number corresponding to the specific heat, in case where it is variable (*i.e.* C_p in $m^2.s^{-2}.K^{-1}$), at the previous time step, in the case of a second-order extrapolation in time. See note below
stored at the cells.

ITSNSA(NPHSMX) [IA] : For each phase, in the case of a calculation run with a second-order discretisation in time with extrapolation of the source terms, property number corresponding to the source term of Navier-Stokes at the previous time step ($kg.m^{-1}.s^{-2}$)
stored at the cells.

ITSTUA(NPHSMX) [IA] : For each phase, in the case of a calculation run with a second-order discretisation in time with extrapolation of the source terms, property number corresponding to the source terms of the turbulence at the previous time step
stored at the cells.

ITSSCA(NPHSMX) [IA] : For each phase, in the case of a calculation run with a second-order discretisation in time with extrapolation of the source terms, property number corresponding to the source terms of the equations solved for the scalars at the previous time step ($kg.m^{-1}.s^{-2}$)
stored at the cells.

IESTIM(NESTMX,NPHSMX) [IA] : For each phase, property number for the NESTMX error estimators for Navier-Stokes. These are currently IESTIM(IESPRE,IPHAS), IESTIM(IESDER,IPHAS), IESTIM(IESCOR,IPHAS), IESTIM(IESTOT,IPHAS)
stored at the cells.

IFLUMA(NVARMX) [IA] : Property number corresponding to the mass flow associated with each variable (*i.e.* for each face of surface S, $\rho \underline{u} . \underline{S}$ in $kg.s^{-1}$). It must be noticed that the mass flows are associated with the variables and not with the phases. This allows to have a distinct convective flow for each scalar.
stored at the internal faces and boundary faces.

IFLUAA(NVARMX) [IA] : Property number corresponding to the mass flow associated with each variable at the previous time step, in the case of a second-order extrapolation in time
stored at the internal faces and boundary faces.

IVISLS(NSCAMX) [IA] : Property number corresponding to the diffusivity of scalars for which it is variable (*i.e.* $\dfrac{\lambda}{C_p}$ for the temperature, in $kg.m^{-1}.s^{-1}$). It must be noticed that the diffusivity is associated with the scalars rather than with the variables. See note below
stored at the cells.

IVISSA(NSCAMX) [IA] : Property number corresponding to the diffusivity of scalars for which it is variable (*i.e.* $\dfrac{\lambda}{C_p}$ for the temperature, in $kg.m^{-1}.s^{-1}$) at the previous time step, in the case of a second-order extrapolation in time
stored at the cells.

ISMAGO(NPHSMX) [IA] : For each phase, property number corresponding to the variable C of the dynamic model, *i.e* so that $\mu_t = \rho C \overline{\Delta}^2 \sqrt{2 S_{ij} S_{ij}}$ (with the notations of [2]). C corresponds to C_s^2 in the classical model of Smagorinsky
stored at the cells.

ICOUR(NPHSMX) [IA] : For each phase, CFL number in each cell at the present time step
stored at the cells.

IFOUR(NPHSMX) [IA] : For each phase, Fourier number in each cell at the present time step

stored at the cells.

IPRTOT(NPHSMX) [IA] : For each phase[16], total pressure in each cell
stored at the cells.

IVISMA(1 or 3) [IA] : When the ALE method for deformable meshes is activated, IVISMA corresponds to the "mesh viscosity", allowing to limit the deformation in certain areas. This mesh viscosity can be isotropic or be taken as a diagonal tensor (depending on the value of the parameter IORTVM.
stored at the cells.

ICMOME(NBMOMX) [IA] : Property number corresponding to the time averages defined by the user. More precisely, it is not the time average that is stored, but a summation over time (the division by the cumulated duration is done just before the results are written)
stored at the cells.

ICDTMO(NBMOMX) [IA] : Property number corresponding to the cumulated duration associated with each time average defined by the user, when this duration is not spatially uniform (see note below)
stored at the cells.

NOTE: VARIABLE PHYSICAL PROPERTIES

Some physical properties such as specific heat or diffusivity are often constant (choice made by the user). In that case, in order to limit the necessary memory, these properties are stored as a simple real number rather than in a domain-sized array of reals.

- It is the case for the specific heat C_p.
  - If C_p is constant for the phase IPHAS, it can be specified in the interface or by indicating ICP(IPHAS)=0 in `usini1`, and the property will be stored in the real number CP0(IPHAS).
  - If C_p is variable, it can be specified in the interface or by indicating ICP(IPHAS)=1 in `usini1`. The code will then modify this value to make ICP(IPHAS) refer to the effective property number corresponding to the specific heat of the phase IPHAS, in a way which is transparent for the user. For each cell IEL, the value of C_p is then given in `usphyv` and stored in the array PROPCE(IEL,IPPROC(ICP(IPHAS))).
- It is the same for the diffusivity K of each scalar ISCAL.
  - If K is constant, it can be specified in the interface or by indicating IVISLS(ISCAL)=0 in `usini1`, and the property will be stored in the real number VISLS0(ISCAL).
  - If K is variable, it can be specified in the interface or by indicating IVISLS(ISCAL)=1 in `usini1`. The code will then modify this value to make IVISLS(ISCAL) refer to the effective property number corresponding to the diffusivity of the scalar ISCAL, in a way which is transparent for the user. For each cell IEL, the value of K is then given in `usphyv` and stored in the array PROPCE(IEL,IPPROC(IVISLS(ISCAL))).

NOTE: CUMULATED DURATION ASSOCIATED WITH THE AVERAGES DEFINED BY THE USER

The cumulated duration associated with the calculation of a time averages defined by the user is often a spatially uniform value. In this case, it is stored in a simple real number: for the mean value IMOM, it is the real number DTCMOM(-IDTMOM(IMOM)) (IDTMOM(IMOM) is negative in this case).
When this cumulated duration is not spatially uniform (for instance in the case of a spatially variable time step), it is stored in PROPCE. It must be noted that the cumulated duration associated with the calculation of the average IMOM is variable in space if IDTMOM(IMOM) is strictly positive. The number of the associated property in PROPCE is then ICDTMO(IDTMOM(IMOM)). For instance, for the

[16] Although the data structure of *Code_Saturne* allows multi-phase variables, the algorithm does not allow more than one pressure

average IMOM, the cumulated duration in the cell IEL will be PROPCE(IEL,ICDTMO(IDTMOM(IMOM))). The user may have a look to the example given in `usproj` to know how to calculate a time averages in a particular cases (printing of extreme values, writing of results, ...).

Two other variables, HBORD and TBORD, should be noted here, although they are relatively local (they appear only in the treatment of the boundary conditions) and are used only by developers.

HBORD(NFABOR) [RA] : Array of the exchange coefficient for temperature (or enthalpy) at the boundary faces. The table is allocated only if ISVHB is set to 1 in `tridim`, which is done automatically but only if the coupling with SYRTHES or the 1D thermal wall module are activated..

TBORD(NFABOR) [RA] : Temperature (or enthalpy) at the boundary faces[17]. The table is allocated only if ISVTB is set to 1 in `tridim`, which is done automatically but only if the coupling with SYRTHES or the 1D thermal wall module are activated..

Tables HBORD and TBORD are of size NFABOR, although they concern only the wall boundary faces.

3.4 Variables related to the numerical methods

The main numerical variables and "pointers"[18] are displayed below.

Boundary conditions

COEFA(NFABOR,*) [RA] : Boundary conditions: see note 2.

COEFB(NFABOR,*) [RA] : Boundary conditions: see note 2.

ICLRTP(NVARMX,2) [IA] : For each variable IVAR (1⩽IVAR⩽NVAR⩽ NVARMX), rank in COEFA and COEFB of the boundary conditions. See note 2.

ICOEF [I] : Rank in ICLRTP of the rank in COEFA and COEFB of the "standard" boundary conditions. See note 2.

ICOEFF [I] : Rank in ICLRTP of the rank in COEFA and COEFB of the "flow" type boundary conditions, reserved for developers. See note 2.

IFMFBR(NFABOR) [IA] : Family number of the boundary faces. See note 1.

IPRFML(NFML,NPRFML) [IA] : Properties of the families of referenced entities. See note 1.

IISYMP [I] : Integer giving the rank in IA of the first element of the section allowing to mark out the "wall" (ITYPFB=IPAROI) or "symmetry" (ITYPFB=ISYMET) boundary faces in order to prevent the mass flow (these faces are impermeable). For instance, for the phase IPHAS, if the face IFAC is a wall or symmetry face, IA(IISMPH+IFAC-1)=0 (with IISMPH=IISYMP+NFABOR*(IPHAS-1)).
Otherwise IA(IISYMP+IFAC-1)=1.
In some subroutines, an array called ISYMPA(NFABOR) allows to simplify the coding with ISYMPA(IFAC)=IA(IISMPH+IFAC-1).

IITRIF [I] : In IA, pointer to ITRIFB.

IITYPF [I] : In IA, pointer to ITYPFB.

[17] It is the physical temeprature at the boundary faces, not the boundary condition for temperature. See [11] for more details on boundary conditions

[18] As for the geometrical variables, some variables may be accessed to directly in sections of the unidimensional macro-arrays IA (for the integers) and RA (for the real numbers) which are present as arguments in every subroutine (apart from a few ones of very low level). The number of the first box of these sections in IA and RA is indicated by an integer stored in a "common". These integers are called "pointers"

ITRIFB(NFABOR,NPHAS) [IA] : Indirection array allowing to sort the boundary faces according to their boundary condition type ITYPFB.

ITYPFB(NFABOR,NPHAS) [IA] : Boundary condition type at the boundary face IFAC for the phase IPHAS (see user subroutine `usclim`).

IUETBO [I] : In RA, pointer to UETBOR, used to store the friction velocity at the wall, in the case of a LES calculation with van Driest-wall damping.

Distance to the wall

IIFAPA(NPHSMX) [IA] : For each phase, the pointer in IA which marks out the number of the wall face(type ITYPFB=IPAROI) which is closest to the center of a given volume when necessary ($R_{ij}-\varepsilon$ with wall echo, LES with van Driest-wall damping, or SST $k-\omega$ turbulence model) and when ICDPAR=2. The number of the wall face (for the phase IPHAS) which is the closest to the center of the cell IEL is therefore IA(IIFAPA(IPHAS)+IEL-1). This calculation method is not compatible with parallelism and periodicity.

IDIPAR [I] : For each phase, pointer in RA to the section allowing to mark out the distance between the center of a given volume and the closest wall, when it is necessary ($R_{ij}-\varepsilon$ with wall echo, LES with van Driest-wall damping, or SST $k-\omega$ turbulence model) and when ICDPAR=1. The distance between the center of the cell IEL and the closest wall is therefore RA(IDIPAR+IEL-1).

IYPPAR [I] : For each phase, pointer in RA to the section allowing to mark out the adimensional distance y^+ between a given volume and the closest wall, when it is necessary (LES with van Driest-wall damping) and when ICDPAR=1. The adimensional distance y^+ between the center of the cell IEL and the closest wall is therefore RA(IYPPAR+IEL-1).

Pressure drops

IICEPD(NPHSMX) [IA] : For each phase IPHAS, pointer in IA to ICEPDC(NCEPDC(IPHAS)), array allowing to mark out the index-numbers of the NCEPDC(IPHAS) cells in which a pressure drop is imposed.
The number of these cells is therefore given by ICEPDC(II)=IA(IICEPD(IPHAS)+II-1), with $1 \leqslant$II$\leqslant$NCEPDC(IPHAS). See the user subroutine `uskpdc`.

ICEPDC(NCEPDC(IPHAS)) [IA] : Number of the NCEPDC(IPHAS) cells in which a pressure drop is imposed. See IICEPD and the user subroutine `uskpdc`.

ICKUPD(NPHSMX) [IA] : For each phase IPHAS, pointer in RA to CKUPDC(NCEPDC(IPHAS),NCKPDC(IPHAS)), array allowing to mark out the NCKPDC(IPHAS) coefficients of the pressure drop tensor of the NCEPDC(IPHAS) cells in which a pressure drop is imposed. See the user subroutine `uskpdc`.

CKUPDC(NCEPDC(IPHAS),NCKPDC(IPHAS)) [RA] : Value of the NCKPDC(IPHAS) coefficients of the pressure drop tensor of the NCEPDC(IPHAS) cells in which a pressure drop is imposed. See ICKPDC and the user subroutine `uskpdc`.

NCEPDC(NPHSMX) [IA] : For each phase, number of cells in which a pressure drop is imposed. See the user subroutine `uskpdc`.

NCKPDC(NPHSMX) [IA] : For each phase, type of the pressure drop tensor (NCKPDC=3: diagonal, NCKPDC=6: non-diagonal). See the user subroutine `uskpdc`.

Mass sources

IICESM(NPHSMX) [IA] : For each phase IPHAS, pointer in IA to ICETSM(NCETSM(IPHAS), array allowing to mark out the numbers of the NCETSM(IPHAS) cells in which a source of mass is imposed. The number of these cells is therefore given by ICETSM(II)=IA(IICESM(IPHAS)+II-1), with 1⩽II⩽NCETSM(IPHAS). See the user subroutine `ustsma`.

IITPSM(NPHSMX) [IA] : For each phase IPHAS, pointer in IA to ITYPSM (type of mass source for each variable). See ITYPSM and the user subroutine `ustsma`.

ICETSM(NCETSM(IPHAS)) [IA] : Number of the NCETSM(IPHAS) cells in which a mass source term is imposed. See IICESM and the user subroutine `ustsma`.

ISMACE(NPHSMX) [IA] : For each phase IPHAS, pointer in RA to SMACEL (mass source term and if necessary injection value for every variable apart from pressure). See SMACEL and the user subroutine `ustsma`.

ITYPSM(NCETSM(IPHAS),NVAR) [IA] : Type of mass source term for each variable (0 for an injection at ambient value, 1 for an injection at imposed value). See the user subroutine `ustsma`.

NCETSM(NPHSMX) [IA] : For each phase, number of cells with mass sources. See the user subroutine `ustsma`.

SMACEL(NCETSM(IPHAS),NVAR) [RA] : Value of the mass source term for pressure. For the other variables, eventual imposed injection value. See the user subroutine `ustsma`.

Wall 1D thermal module

NFPT1D [I] : Number of boundary faces which are coupled with a wall 1D thermal module. See the user subroutine `uspt1d`.

IIFPT1 [I] : In IA, pointer to IFPT1D(NFPT1D), array allowing to mark out the numbers of the NFPT1D boundary faces which are coupled with a wall 1D thermal module. The number of these boundary faces is therefore given by IFPT1D(II)=IA(IIFPT1+II-1), with 1⩽II⩽NFPT1D. See the user subroutine `uspt1d`.

INPPT1 [I] : In IA, pointer to NPPT1D(NFPT1D), array giving the number of discretisation cells in the 1D wall for the NFPT1D boundary faces which are coupled with a wall 1D thermal module. The number of cells for these boundary faces is therefore given by NPPT1D(II)=IA(INPPT1+II-1), with 1⩽II⩽NFPT1D. See the user subroutine `uspt1d`.

IEPPT1 [I] : In IA, pointer to EPPT1D(NFPT1D), array giving the thickness of the 1D wall for the NFPT1D boundary faces which are coupled with a wall 1D thermal module. The wall thickness for these boundary faces is therefore given by EPPT1D(II)=IA(IEPPT1+II-1), with 1⩽II⩽NFPT1D. See the user subroutine `uspt1d`.

Others

DT(NCELET) [RA] : Value of the time step.

IFMCEL(NCELET) [IA] : Family number of the elements. See note 1.

IS2KW(NPHSMX) [IA] : For each phase IPHAS, pointer in RA to the section storing the square of the norm of the deformation rate tensor. In the cell IEL, for the phase IPHAS, $S^2 = 2S_{ij}S_{ij}$ is therefore given by RA(IS2KW(IPHAS)+IEL-1). This array is defined only when the phase IPHASE is treated with the SST $k-\omega$ turbulence model.

IDVUKW(NPHSMX) [IA] : For each phase IPHAS, pointer in RA to the section storing the divergence of the velocity. In the cell IEL, for the phase IPHAS, $div(\underline{u})$ is therefore given by

RA(IDVUKW(IPHAS)+IEL-1). This array is defined only when the phase IPHASE is treated with the SST $k-\omega$ turbulence model (because in this case it may be calculated at the same time as S^2).

NGRMMX [I] : upper limit of the number of grid levels in the case of a multigrid solving (see NGRMAX).

IA(LONGIA) [IA] : Integer work array.

RA(LONGRA) [RA] : Real work array.

NOTE: BOUNDARY CONDITIONS

The boundary conditions in *Code_Saturne* boil down to determine a value for the current variable ϕ at the boundary faces, that is to say ϕ_f, value expressed as a function of $\phi_{I'}$, value of ϕ in I', projection of the center of the adjacent cell on the straight line perpendicular to the boundary face and crossing its center: $\phi_f = A_{\phi,f} + B_{\phi,f}\phi_{I'}$.

For a face IFAC, the pair of coefficients $A_{\phi,f}, B_{\phi,f}$ is stored in COEFA(IFAC,ICLVAR) and COEFB(IFAC,ICLVAR), where the integer ICLVAR=ICLRTP(IVAR,IJCL) determines the rank in COEFA and COEFB of the set of boundary conditions of the variable IVAR.

The second index of the array ICLRTP allows to have several sets of boundary conditions for each variable. The "standard" boundary conditions are determined by IJCL=ICOEF, where ICOEF is a parameter which is fixed automatically by the code, and can be accessed to in the "common" file `numvar.h`. More specificic or advanced boundary conditions can be accessed to with IJCL=ICOEFF.

In practice, for a variable IVAR whose value $\phi_{I'}$ in a boundary cell is known, the value at the corresponding boundary face IFAC is:

ϕ_f=COEFA(IFAC,ICLVAR)+COEFB(IFAC,ICLVAR) $\phi_{I'}$ with ICLVAR=ICLRTP(IVAR,ICOEF)

3.5 User arrays

The code allows to define two user arrays, one integer array and one real array. The default size of these arrays is zero, and may be changed in `usini1`. The two arrays are then passed as arguments in every user subroutine of the code. For instance, a local variable calculated during the determination of the physical properties (user subroutine `usphyv`) may be stored in these arrays and sent to the post-processor at the end of the time step (user subroutine `usvpst`).

NITUSE [I] : Size of the user integer array.

NRTUSE [I] : Size of the user real array.

ITUSER(NITUSE) [IA] : User integer array.

RTUSER(NRTUSE) [RA] : User real array.

3.6 Developer arrays

The code allows to define two developer arrays (similar to the user arrays ITUSER and RTUSER), one integer array a one real array. The default size of these arrays is zero, and may be changed in `usini1`. The two arrays are then passed as arguments in the rest of the code. They are designed to be used during the transitory development phases, in order to ease the tests (transfer of pieces of informations without consequence on the arguments of the subroutines).

NIDEVE [I] : Size of the developer integer array.

NRDEVE [I] : Size of the developer real array.

IDEVEL(NIDEVE) [IA] : Complementary integer array, used during development and test phases.

RDEVEL(NRDEVE) [RA] : Complementary real array, used during development and test phases.

3.7 Parallelism and periodicity

Activation

Parallelism and periodicity are activated by means of the launch script in the standard cases:

- On clusters with PBS batch systems (like the EDF R&D Chatou cluster), the launching of a parallel run requires to complete the `PBS` batch cards located in the beginning of `lance`, and particularly to set the number of physical nodes (`nodes`) and the number of physical processors per node (`ppn`) wanted. This can be done through the Graphical Interface or by editing the `lance` file directly. The number of processors used for the calculation will then be set automatically to the number of processors reserved and the variable `NOMBRE_DE_PROCESSEURS` can be left empty (see also §2.6).
- On clusters with LSF batch systems (like the CCRT machines), the launching of a parallel run requires to complete the `LSF` batch cards located in the beginning of `lance`, and particularly to set the number of processors (`#BSUB -n`) wanted and the limit CPU time (`#BSUB -W`). As for now, this can only be done by editing the `lance` file directly. The number of processors used for the calculation will then be set automatically to the number of processors reserved and the variable `NOMBRE_DE_PROCESSEURS` can be left empty (see also §2.6).
- On clusters with other batch systems, `lance` file may have to be modified manually. Please do not hesitate to contact the *Code_Saturne* support (saturne-support@edf.fr) so that these modifications can be added to the standard launch script to make it more general.
- Although on batch systems the `NOMBRE_DE_PROCESSEURS` variable in the script (indicating the number of processors used for the calculation) is filled automatically to the number of processors reserved, the user can still choose to specify another value for it. This might only happen in very specific conditions and is not advised, as it will probably not be compatible with the batch system. Indeed, batch systems forbid to launch a calculation on more processors than the number of processors reserved, and some batch systems also forbid to launch a calculation on less processors than the number of processors reserved (automatic timeout on the idle processors that will stop the whole calculation).
- Periodicity is activated through the Graphical Interface or by completing the `COMMANDE_PERIO` of the launch script `lance`. The transformation allowing to pass from a boundary to the other one must be defined (the direction does not matter) and the set of periodical faces should be (optional but strongly advised) marked out (for instance by means of a color).
- Periodicity is compatible with parallelism.
- Periodicity can also work when the periodic boundaries are meshed differently (periodicity of non-conforming faces), *apart* from the case of a 180 degree rotation periodicity with faces couples on the rotation axis.
- A parallel calculation may be stopped in the same manner as a sequential one using a `ficstp` file (see praragraph 2.2.4).
- The standard pieces of information displayed in the listing (marked out with `'v '` for the min/max values of the variables), `'c '` for the data concerning the convergence and `'a '` for the values before clipping) are global values for the whole domain and not related to each processor.

User subroutines

The user can notice in a subroutine

- that the presence of periodicity is tested with the variable IPERIO (=1 if periodicity is activated);

- that the presence of rotation periodicities is tested with the variable IPEROT (number of rotation periodicities);
- that the parallel running of a calculation is tested with the variable IRANGP (IRANGP is worth -1 in the case of a non-parallel calculation and N-1 in the case of a parallel calculation, N being the number of the current processor)

Attention must be paid to the coding of the user subroutines. If conventionnal subroutines like `usini1` or `usclim` usually do not cause any problem, some kind of developments are more complicated. The most usual cases are dealt with below.
Examples are given in the subroutine `usproj`.

- **Access to information related to neighboring cells in parallel and periodic cases**.
  When periodicity or parallelism are brought into use, some cells of the mesh become physically distant from their neighbors. Concerning parallelism, the calculation domain is split and distributed between the processors: a cell located at the "edge" of a given processor may have neighbors on different processors.
  In the same way, in case of periodicity, the neighboring cells of cells adjacent to a periodic face are generally distant.
  When data concerning neighboring cells are required for the calculation, they must first be searched on the other processors or on the other edge of periodic frontiers. In order to ease the manipulation of these data, they are stored temporarily in virtual cells called "halo" cells, as can be seen in figure 1. It is in particular the case when the following operations are made on a variable A:
  - calculation of the gradient of A (use of `grdcel`);
  - calculation of an internal face value from the values of A in the neighboring cells (use of IFACEL).

  The variable A needs to be exchanged before these operations can be made: to allow it, the subroutines `parcom` and `percom` need to be called **in this order**.
- **Global operations in parallel mode**.
  In parallel mode, the user must pay attention during the realisation of global operations. The following list is not exhaustive:
  - calculation of extreme values on the domain (for instance, minimum and maximum of some calculation values);
  - test of the existence of a certain value (for instance, do faces of a certain color exist ?);
  - verification of a condition on the domain (for instance, is a given flow value reached somewhere ?);
  - counting out of entities (for instance, how many cells have pressure drops ?);
  - global sum (for instance, calculation of a mass flow or the total mass of a pollutant).

  The user may refer to the different examples present in the user subroutine `usproj`.
  Care should be taken with the fact that the frontiers between subdomains consist of **internal** faces shared between two processors (these are indeed internal faces, even if they are located at a "processor edge"). They should not be counted twice (once per processor) during global operations about internal faces (for instance, counting the internal faces per processor and summing all the obtained numbers drives into overevaluing the number of internal faces of the initial mesh).
- **The writing ; operations that should be made on one processor in parallel mode**.
  In parallel mode, the user must pay attention during the writing of pieces of information. The writing of pieces of information in the listing can be done simply by using the logic unit NFECRA (each processor will write in its own listing file): use `WRITE(NFECRA,...`.

If the user wants an operation to be done by only one processor (for example, open or write a file), the associated instructions must be included inside a test on the value of IRANGP (generally it is the processor 0 which realises these actions, and we want the subroutine to work in non-parallel mode, too: `IF (IRANGP.LE.0) THEN ...`).

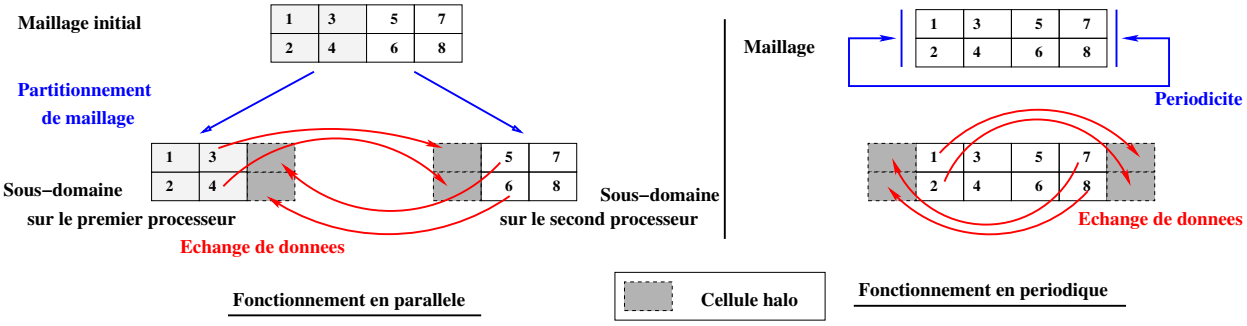

Figure 1: Periodicity and parallelism: exchange structure.

Some notes about the periodicity

Some particular points should be reminded:

- periodicity is incompatible with
  - multigrid algorithm,
- rotation periodicity is incompatible with
  - semi-transparent radiation,
  - reinforced velocity-pressure coupling (IPUCOU=1).
- although it has not been the case so far, potential problemes might be met in the case of rotation periodicity with the LRR $R_{ij} - \varepsilon$ model. They would come from the way of taking into account the orthotrope viscosity (however, this term has usually a low influence).

3.8 Geometric and particulate arrays related to lagrangian modeling

In this section is given a non-exhaustive list of the main variables which may be seen by the user in the lagrangian module. Most of them should not be modified by the user. They are calculated automatically from the data. However it may be useful to know their meaning.

These variables are listed in the alphabetical index in the end of this document.

The type of each variable is given: integer [I], real number [R], integer array [IA], real array [RA].

Size of the lagrangian arrays

LNDNOD [I] : Size of the array ICOCEL concerning the cells-faces connectivity (the faces-nodes connectivity needs to be given to allow the construction of this connectivity. See note 3 of section 3.1).

NBPMAX [I] : Maximum number of particles simultaneously acceptable in the calculation domain.

NVP [I] : Number of variables describing the particles for which a stochastic differential equation (SDE) is solved.

NVLS [I] : Number of variables describing the supplementary user particles for which a SDE is solved.

NVEP [I] : Number of real state variables describing the particles.

NIVEP [I] : Number of integer state variables describing the particles.

NTERSL [I] : Number of source terms representing the backward coupling of the dispersed phase on the continuous phase.

NVLSTA [I] : Number of volumetric statistical variables .

NVLSTS [I] : Number of supplementary user volumetric statistical variables.

NVISBR [I] : Number of boundary statistical variables.

NUSBOR [I] : Number of supplementary user boundary statistical variables.

NVGAUS [I] : Number of gaussian random variables.

Note: continuous eulerian phase number

The current version of lagrangian module is planned to work with only one eulerian phase. This phase carries inclusions, and source terms of backward coupling are applied to it, if necessary. The number of this phase is stored in the variable ILPHAS. The standard value is ILPHAS = 1.

Lagrangian arrays

ICOCEL(LNDNOD) [IA] : Cells - internal/boundary faces connectivity. The numbers of the boundary faces are marked out in ICOCEL with a negative sign.

ITYCEL(NCELET+1) [IA] : Array containing the position of the first face surrounding every cell in the array ICOCEL (see subroutine `lagdeb` for more details).

ETTP(NBPMAX,NVP) [RA] : Variables forming the state vector related to the particles: either at the current stage if the lagrangian scheme is a second-order, or at the current time step if the scheme is a first-order. These variables are marked out by "pointers" whose value can vary between 1 and NVP:

→ JMP: particle mass

→ JDP: particle diameter

→ JXP, JYP, JZP: particle coordinates

→ JUP, JVP, JWP: particle velocity components

→ JUF, JVF, JWF: locally undisturbed fluid flow velocity components

→ JTP, JTF: particle and locally undisturbed fluid flow temperature (°C)

→ JCP: particle specific heat

→ JHP: coal particle temperature (°C)

→ JMCH: mass of reactive coal of the coal particle

→ JMCK: mass of coke of the coal particle

→ JVLS(II): II*th* supplementary user variable

ETTPA(NBPMAX,NVP) [RA] : Variables forming the state vector related to the particles: either at the previous stage if the lagrangian scheme is a second-order, or at the previous time step if the lagrangian scheme is a first-order.

ITEPA(NBPMAX,NIVEP) [IA] : Integer state variables related to the particles. They are marked out by the following "pointers":

→ JISOR: Number of the current cell containing the particle; this number is reactualised during the trajectography step

→ JINCH: Number of the coal particle

TEPA(NBPMAX,NVEP) [RA] : Real state variables related to the particles. They are marked out by the following "pointers":

→ JRTSP: particle residence time

→ JRPOI: particle statistic weight

→ JRDCK: coal particle shrinking core diameter

→ JRD0P: coal particle initial diameter

→ JRR0P: coal particle initial density

INDEP(NBPMAX) [IA] : Storage of the cell number of every particle at the beginning of a lagrangian iteration ; this data is not modified during the iteration.

VITPAR(NBPMAX,3) [RA] : At the beginning of the trajectography, VITPAR contains the particle velocity vector components; the modifications of the particle velocity following every particle/boundary interaction are saved in this array ; after the trajectography and backward coupling steps, ETTP is updated with VITPAR.

VITFLU(NBPMAX,3) [RA] : At the beginning of the trajectography, VITFLU contains the locally undisturbed fluid flow velocity vector components; the modifications of the locally undisturbed fluid flow velocity following every particle/boundary interaction are saved in this array ; after the trajectography and backward coupling steps, ETTP is updated with VITFLU.

GRADPR(NCELET,3) [RA] : Pressure gradient of the continuous phase.

GRADVF(NCELET,9) [RA] : Gradient of the continuous phase fluid velocity (useful if the complete model is activated: see MODCPL).

CPGD1(NBPMAX) [RA] : First devolatilisation term (light volatile matters) of the coal particles (useful in the case of backward coupling on the continuous phase).

CPGD2(NBPMAX) [RA] : Second devolatilisation term (heavy volatile matters) of the coal particles (useful in the case of backward coupling on the continuous phase).

CPGHT(NBPMAX) [RA] : Heterogeneous combustion term of the coal particles (useful in the case of backward coupling on the continuous phase).

STATIS(NCELET,NVLSTA) [RA] : Volumetric statistics related to the dispersed phase; these statistics are the kind of results expected with the lagrangian module. It is from these statistics that we obtain information concerning the particle cloud (the particle trajectories should only be observed on "pedagogical" account); they are marked out by the following "pointers":

→ ILVX,ILVY,ILVZ: mean dispersed phase velocity

→ ILVX2,ILVY2,ILVZ2: dispersed phase velocity standard deviation

→ ILFV: dispersed phase volumetric concentration

→ ILPD: sum of the statistical weights

→ ILTP: dispersed phase temperature (°C)

→ ILDP: dispersed phase mean diameter

→ ILMP: dispersed phase mean mass

→ ILHP: temperature of the coal particle cloud (°C)

→ ILMCH: mass of reactive coal of the coal particle cloud

→ ILMCK: mass of coke of the coal particle cloud

→ ILMDK: shrinking core diameter of the coal particle cloud

→ ILVU(II): II*th* supplementary user volumetric statistics

PARBOR(NFABOR,NVISBR) [RA] : Boundary statistics related the dispersed phase ; after every particle/boundary interaction it is possible to save some data and to calculate averages ; the boundary statistics are marked out by the following "pointers":

→ INBR: number of particle/boundary interactions

→ IFLM: particle mass flow at the boundary faces

→ IANG: mean interaction angle with the boundary faces (see example in `uslabo`)

→ IVIT: mean interaction velocity with the boundary faces

→ IENC: mass of coal deposit at the walls

→ IUSB(II): II*th* supplementary user boundary statistics

TSLAGR(NCELET,NTERSL) [RA] : Source terms corresponding to the backward coupling of the dispersed phase on the continuous phase. These source terms are marked out by the following "pointers":

→ ITSVX, ITSVY, ITSVZ: explicit source terms for the continuous phase velocity

→ ITSLI: implicit source term for the continuous phase velocity and for the turbulent energy if the $k-\varepsilon$ model is used

→ ITSKE: explicit source term for the turbulent dissipation and the turbulent energy if the $k-\varepsilon$ turbulence model is used for the continuous phase

→ ITSR11,... ITSR33: source terms for the Reynolds stress and the turbulent dissipation if the $R_{ij}-\varepsilon$ turbulence model is used for the continuous phase

→ ITSMAS: mass source term

→ ITSTE, ITSTI: explicit and implicit thermal source terms for the thermal scalar of the continuous phase

→ ITSMV1(ICHA), ITSMV2(ICHA): source terms respectively for the light and heavy volatile matters

→ ITSCO: source term for the carbon released during heterogeneous combustion

→ ITSF: source term for the air variance (not used at the present time)

CROULE(NCELET) [TR] : Importance function for the technique of variance reduction (cloning/fusion of particles).

VAGAUS(NBPMAX,NVGAUS) [RA] : Vectors of gaussian random variables.

AUXL(NBPMAX,3) [RA] : Auxiliary work array.

3.9 Variables saved to allow calculation restarts

The directory `SUITE*` contains:

- `suiava`: main restart file,
- `suiavx`: auxiliary restart file (see ILEAUX, IECAUX),
- `rayava`: restart file for the radiation module,
- `lagava`: main restart file for the lagrangian module,
- `lasava`: auxiliary restart file for the lagrangian module (mainly for the statistics),
- `t1dava`: restart file for the 1D wall thermal module,
- `vorava`: restart file for the vortex method (see IVRTEX).

The main restart file contains the values in every cell of the mesh for pressure, velocity, turbulence variables and scalars. Its content is sufficient for a calculation restart, but the complete continuity of the solution at restart is not ensured[19].

The auxiliary restart file completes the main restart file to ensure solution continuity in the case of a calculation restart. If the code cannot find one or several pieces of data required for the calculation restart in the auxiliary restart file, default values are then used. This allows in particular to run calculation restarts even if the number of faces has been modified (for instance in case of modification of the mesh merging or of the periodicity conditions[20]). More precisely, the auxiliary restart file contains the following data:

- type and value of the time step, turbulence model,
- density value at the cells and boundary faces, if it is variable,
- values at the cells of the other variable physical properties, when they are extrapolated in time (molecular dynamic viscosity, turbulent or subgrid scale viscosity, specific heat, scalar diffusivities); for the Joule effect, the specific heat is stored automatically (in case the user should need it at restart to calculate the temperature from the enthalpy before the new specific heat has been estimated),
- time step value at the cells, if it is variable,
- mass flow value at the internal and boundary faces (at the last time step, and also at the previous time step if required by the time scheme),

[19] in other words, a restart calculation of n time steps following a calculation of m time steps will not yield strictly the same resluts as a direct calculation on m+n time steps, whereas it is the case when the auxiliary file is used

[20] imposing a periodicity changes boundary faces into internal faces

- boundary conditions,
- values at the cells of the source terms when they are extrapolated in time,
- number of time-averages, and values at the cells of the associated cumulated values,
- for each cell, distance to the wall when it is required (and index-number of the nearest boundary face, depending on ICDPAR),
- values at the cells of the external forces in balance with a part of the pressure (hydrostatic, in general),
- for the D3P gas combustion model: massic enthalpies and temperatures at entry, type of boundary zones and entry indicators,
- for the EBU gas combustion model: temperature of the fresh gas, constant mixing rate (for the models without mixing rate transport), types of boundary zones, entry indicators, temperatures and mixing rates at entry,
- for the LWC gas combustion model: the boundaries of the probability density functions for enthalpy and mixing rate, types of boundary zones, entry indicators, temperatures and mixing rates at entry,
- for the pulverised coal combustion: coal density, types of boundary zones, variables IENTAT, IENTCP, TIMPAT, X20 (in case of coupling with the lagrangian module, IENCP and X20 are not saved),
- for the electric module: the tuned potential difference DPOT and, for the electric arc module, the tuning coefficient COEJOU (when the boundary conditions are tuned), the Joule source term for the enthalpy (with the Joule effect is activated) and the Laplace forces (with the electric arc module).

It should be noted that, if the auxiliary restart file is read, it is possible to run calculation restarts with relaxation of the density[21](when it is variable), because this variable is stored in the restart file. On the other hand, it is generally not possible to do the same with the other physical properties (they are stored in the restart file only when they are extrapolated in time, or with the Joule effect for the specific heat).

When reading `suiava`, `suiavx`, `rayava`, `lagava`, `lasava` or `t1dava`, the file format (binary or ASCII) is automatically determined by the code. When writing these files, the format can be specified by the user (see IFOAVA, IFOAVX, IFOAVR, IFOAVL, IFOVLS and IFOVT1). The file `vorava` has a different structure from the other ones and is always in ASCII. Therefore there is no variable to specify its format.

In the case of parallel calculations, it should be noted that all the processors will write their restart data in the same files. Hence, for instance, there will always be one and only one `suiava` file, whatever the number of processors used. The data in the file are written according to the initial full domain index-numbers for the cells, faces and nodes. This allows in particular to continue with p processors a calculation begun with n processors, or to make the restart files independent of any vectorial renumbering that may be carried out in each domain.

On the other hand, if the numbering of the initial full domain mesh is modified, the restart files will not be compatible. This may be the case if the mesh is composed of different elements that are pasted by the Preprocessor module and the order of the different elements has been changed in the Preprocessor command line between two calculations.

WARNING: if the mesh is composed of several files, the order in which they appear in the launch script or in the Graphical Interface must not be modified in case of a calculation restart[22].

[21] such a relaxation only makes sense for a stationary calculation

[22] when uncertain, the user can check the saved copy of the launch script in the `RESU` directory, or the head of the `listpre` file, which repeats the command line passed to the Preprocessor module

NOTE : when meshes are pasted by the Preprocessor module with potential hanging nodes, two nodes closer than a certain (small) tolerance will be merged. Hence, due to numerical round-up errors, two different machines may yield different results. This might change the number of faces in the global domain[23] *and make restart files incompatible. Should that problem arise when making a calculation restart on a different architecture, the solution is to discard the* ***suiavx*** *file and use only the* ***suiava*** *file.*

4 User subroutines

4.1 Preliminary comments

The user can run the calculations with or without an interface, with or without the user subroutine. Without interface, some user subroutines are needed. With interface, all the user subroutines are optional.

The parameters can be read in the interface and then in the user subroutine. In the case that a parameter is specified in the interdace and in the user subroutine, it is the value in the user subroutine that is taken into acount. It is for that reason that all the examples of user subroutines are placed in the `USERS` directory by the case preparer `cree_sat`.

4.2 Using selection criteria in user subroutines

In order to use selection criteria (cf. §2.8) in Fortran user subroutines, a collection of utility subroutines is provided. The aim is to define a subset of the mesh, for example:

- boundary regions (cf. `usclim`, `uscpcl`, `usray2`, `uslag2`,...),
- volumic initialization (cf. `usiniv`,...),
- porosity region (cf. `uskpdc`),
- source terms region (cf. `ustsns`, `ustssc`),
- advanced post-processing (cf. `usdpst`), `usproj`, ...),

This section explains how to define surface or volume sections, in the form of lists `LSTELT` of `NLELT` elements (internal faces, boundary faces or cells). For each type of element, the user calls the appropriate Fortran subroutine: `getfbr` for boundary faces, `getfac` for internal faces and `getcel` for cells. All of these take the three following arguments:

- the character string which contains the selection criterion (see some examples below),
- the returned number of elements `NLELT`,
- the returned list of elements `LSTELT`.

Several examples of possible selections are given here:

- `CALL GETFBR('Face_1, Face_2', NLELT, LSTELT)` to select boundary faces in groups Face_1 or Face_2,
- `CALL GETFAC('4', NLELT, LSTELT)` to select internal faces of color 4,
- `CALL GETFAC('not(4)', NLELT, LSTELT)` to select internal faces which have a different color from 4,

[23] the number of cells will not be modified, it is always the sum of the number of cells of the different meshes

- `CALL GETFAC('4 to 8', NLELT, LSTELT)` to internal faces with color between 4 and 8 internal faces,
- `CALL GETCEL('1 or 2', NLELT, LSTELT)` to select cells with colors 1 or 2,
- `CALL GETFBR('1 and Y > 0', NLELT, LSTELT)` to select boundary faces of color 1 which have the coordinate $Y > 0$,
- `CALL GETFAC('normal[1, 0, 0, 0.0001]', NLELT, LSTELT)` to select internal faces which have a normal direction to the vector (1,0,0),
- `CALL GETCEL('all[]', NLELT, LSTELT)` to select all cells.

The user may then use a loop on the selected elements. For instance, in the subroutine `usclim` used to impose boundary conditions, let us consider the boundary faces of color number 2 and which have the coordinate $X <= 0.01$ (so that `CALL GETFBR('2 and X <= 0.01', NLELT,LSTELT)`); we can do a loop (`DO ILELT = 1, NLELT`) and obtain `IFAC = LSTELT(ILELT)`.

NOTE: LEGACY METHOD USING EXPLICIT FAMILIES AND PROPERTIES

The selection method for user subroutines by prior versions of *Code_Saturne* is still available, though it may be removed in future versions. This method was better adpated to working with colors than with groups, and is explained here:

From *Code_Saturne*'s point of view, all the references to mesh entities (boundary faces and volume elements) correspond to a number (color number or negative of group number) associated with the entity. An entity may have several references (for instance, one entity may have one color and belong to several groups). In *Code_Saturne*, these references may be designated as "properties".
The mesh entities are gathered in equivalence classes on the base of their properties. These equivalence classes are called "families". All the entities of one family have the same properties. In order to know the properties (in particular the color) of an entity (a boundary face for example), the user must first determine the family to which it belongs.
For instance, let's consider a mesh whose boundary faces have all been given one color (for example using SIMAIL). The family of the boundary face IFAC is IFML=IFMFBR(IFAC). The first (and only) property of this family is the color ICOUL, obtained for the face IFAC with ICOUL=IPRFML(IFML,1). In order to know the property number corresponding to a group, the user may refer to the listing of the Preprocessor (not forgetting to use the negative of the number in this case), or use the utility function `NUMGRP(NOMGRP, LNGNOM)` (with a name `NOMGRP` of the type `CHARACTER*` and its lenght `LNGNOM` of the type `INTEGER`).

4.3 Initialisation of the main key words: `usini1`

Subroutine only called during calculation initialisation.

This subroutine is used to indicate the value of different calculation basic parameters: constant and uniform physical values, parameters of numerical schemes, input-output management ...

In the case of a calculation launched using the interface, it is only used to modify high-level parameters which can not be managed by the interface. In the case of a code utilisation without interface, this subroutine is compulsory and all the headings must be completed.

For more details about the different parameters, please refer to the key word list (§5).

`usini1.F` is in fact a gouping of 6 sperate subroutines: `usipph`, `usinsc`, `usipsc`, `usipgl`, `usipsu`and `usipes`. Each one controls the management of various specific parameters. The key words that dont' feature in the supplied example can be provided by the user in `FORT/USERS/base`; in this case,

understanding of the comments is needed to add the key words in the appropriate subroutine (the most widely used is IPHAS, it will assure that the value has been well defined). The modifiable parameters in each of the subroutines of `usini1.F` are:

- `usipph`: ITURB and ICP (don't modify these parameters anywhere else)
- `usinsc`: NSCAUS (don't modify these parameters anywhere else)
- `usipsc`: ISCAVR and IVISLS (don't modify these parameters anywhere else)
- `usipgl`: IDTVAR, IPUCOU, IPHYDR and the parameters related to the error estimators(don't modify these parameters anywhere else).
- `usipsu`: physical parameters of the calculation (thermal scalar, physical properties,...), numeric parameters (time steps, number of iterations,..),definition of the time averages.
- `usipes`: post treatment display parameters (periodicity, variable names, position of probes,...)

For more details of the different parameters, see the list of key words (§5). The names of the key words can also be seen in the helps sections of the interface.

NOTES

• Determined in the list of NSCAUS user scalars, representing the mean square fluctuations of another whilst informing the ISCAVR array (warning, this was not the case in version 1.0). For the other scalars, ISCAVR does not need to be completed (by default, ISCAVR(II)$\leqslant$0). For instance, if the scalar JJ represents the average of the square of the fluctuations of the scalar KK, the user must indicate ISCAVR(JJ)=KK (1$\leqslant$KK$\leqslant$NSCAUS).

• When using the interface, only the supplementary parameters (which can not be defined in the interface) should appear in `usini1`. To spare the user the necessity to delete the other parameters appearing as examples in the subroutine, the utility program `cree_sat` comments automatically all the example lines of `usini1` with a code `Cex`. The user needs then only to uncomment the lines which are useful in his case. This function of `cree_sat` can be inactivated with the option `-noihm` (useful if the user knows that he will not use the interface).

4.4 Management of boundary conditions: `usclim`

Subroutine called every time step.

It is the second compulsory subroutine for every calculation launched without interface(except in the specific physics case where the corresponding boundary condition user subroutine must be used)
When the interface is used, `usclim` is used to define complex boundary conditions (input profiles, conditions varying in time, ...) which could not be specified by means of the interface, and only these need to be defined. In the case of a calculation launched without the interface, all the boundary conditions must appear in `usclim`.
`usclim` is essentially constituted of a loop on the boundary faces. Several sequences of `CALL GETFBR ('criterion', NLELT, LSTELT)` (cf. §4.2) allows to differentiate the boundary faces according to their group(s), their color(s) or geometrical criterion(s). If needed, disposal geometric and physical variables are also available to the user, these allow him to differentiate the boundary faces using other criterions.

For more details about the treatment of boundary conditions, the user may refer to the theoretical and computer documentation [11] of the subroutine `condli` (for the wall conditions, see `clptur`) (to access to this document on a workstation, use `info_cs noyau`).

From the user point of view, the boundary conditions are totally determined by three arrays[24] : ITYPFB(NFABOR,NPHAS), ICODCL(NFABOR,NVAR) and RCODCL(NFABOR,NVAR,3).

[24] except with lagrangien

- ITYPFB(IFAC,IPHAS) defines the type of the face IFAC (input, wall ...) for the phase IPHAS.
- ICODCL(IFAC,IVAR) defines the type of boundary condition for the variable IVAR at the face IFAC (Dirichlet, flow ...).
- RCODCL(IFAC,IVAR,.) gives the numerical values associated with the type of boundary condition (value of the Dirichlet, of the flow ...).

In the case of standard boundary conditions (see §4.4.1), it is enough to complete ITYPFB(IFAC,IPHAS) and some boxes of the array RCODCL, the array ICODCL and most of the boxes of RCODCL are completed automatically. For non-standard boundary conditions (see §4.4.2), the arrays ICODCL and RCODCL must be totally completed.

4.4.1 Coding of standard boundary conditions

The standard values taken by the indicator ITYPFB are: IENTRE, IPAROI, ISYMET, ISOR09, ISOR10 and IINDEF.

- If ITYPFB=IENTRE: inlet face.

  → Zero flow condition for pressure and Dirichlet condition for all other variables. The value of the Dirichlet must be given in RCODCL(IFAC,IVAR,1) for every value of IVAR, apart from IVAR=IPR(IPHAS). The other boxes of RCODCL and ICODCL are completed automatically.

- If ITYPFB=IPAROI: solid wall face, impermeable and with friction.

  → the eventual moving velocity of the wall tangent to the face is given by RCODCL(IFAC,IVAR,1) (IVAR being IU(IPHAS), IV(IPHAS) or IW(IPHAS)). The initial value of RCODCL(IFAC,IVAR,1) is zero for the three velocity components (and therefore needs to be specified only in the case of the existence of a slipping velocity).
  WARNING: the wall moving velocity must be in the boundary face plane. By security, the code uses only the projection of this velocity on the face. As a consequence, if the velocity specified by the user is not in the face plane, the wall moving velocity really taken into account will be different.

  → Concerning the scalars, two kinds of boundary conditions can be defined:

  ⇝ Imposed value at the wall. The user must write
  ICODCL(IFAC,IVAR)=5
  RCODCL(IFAC,IVAR,1)=imposed value

  ⇝ Imposed flow at the wall. The user must write
  ICODCL(IFAC,IVAR)=3
  RCODCL(IFAC,IVAR,3)=flow imposed value (for the flow definition according to the variable, the user may refer to the case ICODCL=3 of the paragraph 4.4.2).

  ⇝ If the user does not complete these arrays, the default condition is zero flow.

- If ITYPFB=ISYMET: symmetry face (or wall without friction)

  → Nothing to write in ICODCL and RCODCL.

- If ITYPFB=ISOR09: "zero flow" outlet face

  → If the mass flow is going out, zero flow condition for the scalars (apart from pressure) and the velocity.

  → If the mass flow is coming in, zero flow condition for the scalars (apart from pressure) and the value zero is imposed to the velocity at the face (but not to the mass flow).

→ In both cases the boundary condition type for pressure is a Dirichlet, calculated in order to have $\frac{d}{dn}\left(\frac{dP}{d\tau}\right) = 0$. The pressure is given the value P_0 at the first face ISOR09 met(the fixed reference is always linked to just 1 face, even if there are several exits).

→ Nothing to write in ICODCL or RCODCL.

- If ITYPFB=ISOR10: "entering Dirichlet" outlet face

→ If the mass flow is going out, zero flow condition for the scalars (apart from pressure) and the velocity.

→ If the mass flow is coming in, Dirichlet condition for the scalars and the value zero is imposed to the velocity at the face (but not to the mass flow).

→ In both cases, the boundary condition type for pressure is a Dirichlet, calculated in order to have $\frac{d}{dn}\left(\frac{dP}{d\tau}\right) = 0$. The pressure is given the value P_0 at the first face ISOR09 met. The pressure drop is always linked to just 1 face, even is there are several exits.

→ RCODCL(IFAC,IVAR,1) must be completed to give the value of the Dirichlet for every scalar apart from pressure. In the case of the $R_{ij} - \varepsilon$ model, the value zero will be given to the extra-diagonal terms of the stress tensor.

- Si ITYPFB=IINDEF: non-defined type face (non-standard case)

→ The coding is done by completing every array RCODCL and ICODCL (see §4.4.2).

NOTES

• Whatever the value of the indicator ITYPFB(IFAC,IPHAS), if the array ICODCL(IFAC,IVAR) is modified by the user (*i.e.* filled in by a value different from zero), the code will not use the default conditions for the variable IVAR at the face IFAC, but will take into account the values of ICODCL and RCODCL given by the user (these arrays must then be totally completed, like in the non-standard case).
For instance, for a symmetry face at which the scalar 1 is given a Dirichlet condition equal to 23.8 (with an infinite exchange coefficient):

```
ITYPFB(IFAC,IPHAS)=ISYMET
ICODCL(IFAC,ISCA(1))=1
RCODCL(IFAC,ISCA(1),1)=23.8D0
```

(`RCODCL(IFAC,ISCA(1),2)=RINFIN` is the default value, so it is not necessary to specify it)
The boundary conditions for the other variables are still automatically defined.

• The user may define new types of wall faces. He only needs to choose a value N and to specify completely the boundary conditions corresponding to this new wall face type (see §4.4.2). He must then specify ITYPFB(IFAC,IPHAS)=N. The value of N must be between 1 and NTYPMX (maximum number of boundary face types), and of course different from the values IENTRE, IPAROI, ISYMET, ISOR09, ISOR10 and IINDEF (the value of these variables is given in the file `paramx.h`). This allows to isolate easily some boundary faces, in order to calculate balances.

4.4.2 Coding of non-standard boundary conditions

In the case of a face not corresponding to a standard type, the user must complete all of the arrays ITYPFB, ICODCL and RCODCL. ITYPFB(IFAC,IPHAS) is then worth IINDEF or another value defined by the user (see note in the end of paragraph 4.4.1). The arrays ICODCL and RCODCL must be completed as follows:

- If ICODCL(IFAC,IVAR)=1: Dirichlet condition at the face IFAC for the variable IVAR.

→ RCODCL(IFAC,IVAR,1) is the value of the variable IVAR at the face IFAC.

→ RCODCL(IFAC,IVAR,2) is the value of the exchange coefficient between the outside and the fluid for the variable IVAR. An infinite value (`RCODCL(IFAC,IVAR,2)=RINFIN`) indicates a perfect transfer between the outside and the fluid (default case).

→ RCODCL(IFAC,IVAR,3) is not used.

→ RCODCL(IFAC,IVAR,1) is expressed in the unit of the variable IVAR, *i.e.*:

⇝ m/s for the velocity
⇝ m^2/s^2 for the Reynolds stress
⇝ m^2/s^3 for the dissipation
⇝ Pa for the pressure
⇝ °C for the temperature
⇝ $J.kg^{-1}$ for the enthalpy
⇝ $°C^2$ for the temperature fluctuations
⇝ $J^2.kg^{-2}$ for the enthalpy fluctuations

→ RCODCL(IFAC,IVAR,2) is expressed in the following unit (defined so that by multiplying the exchange coefficient and the variable, the obtained flow has the same unit as the flow defined below for ICODCL=3):

⇝ $kg.m^{-2}.s^{-1}$ for the velocity
⇝ $kg.m^{-2}.s^{-1}$ for the Reynolds stress
⇝ $s.m^{-1}$ for the pressure
⇝ $W.m^{-2}.°C^{-1}$ for the temperature
⇝ $kg.m^{-2}.s^{-1}$ for the enthalpy

- If ICODCL(IFAC,IVAR)=3: flow condition at the face IFAC for the variable IVAR.

→ RCODCL(IFAC,IVAR,1) and RCODCL(IFAC,IVAR,2) are not used.

→ RCODCL(IFAC,IVAR,3) is the flow value of IVAR at the wall. This flow is negative if it is a source for the fluid. It corresponds to:

⇝ $-C_p(\dfrac{\lambda_T}{C_p}+\dfrac{\mu_t}{\sigma_T})\underline{\text{grad}}\ T\cdot\underline{n}$ in the case of a temperature (in W/m^2).
$-(\lambda_h+\dfrac{\mu_t}{\sigma_h})\underline{\text{grad}}\ h\cdot\underline{n}$ in the case of an enthalpy (in W/m^2).
$-(\lambda_\varphi+\dfrac{\mu_t}{\sigma_\varphi})\underline{\text{grad}}\ \varphi\cdot\underline{n}$ in the case of another scalar φ (in $kg.m^{-2}.s^{-1}.[\varphi]$, where $[\varphi]$ is the unit of φ).
⇝ $-\Delta t\ \underline{\text{grad}}\ P\cdot\underline{n}$ in the case of the pressure (in $kg.m^{-2}.s^{-1}$).
⇝ $-(\mu+\mu_t)\underline{\text{grad}}\ U_i\cdot\underline{n}$ in the case of a velocity component (in $kg.m^{-1}.s^{-2}$).
⇝ $-\mu\underline{\text{grad}}\ R_{ij}\cdot\underline{n}$ in the case of a R_{ij} tensor component (in W/m^2).

- If ICODCL(IFAC,IVAR)=4: symmetry condition, for the symmetry faces or wall faces without friction. This condition can only be used for the velocity components ($\underline{U}\cdot\underline{n}=0$) and the R_{ij} tensor components (for the other variables, a zero flow condition type is generally used).

- If ICODCL(IFAC,IVAR)=5: friction condition, for the wall faces with friction. This condition can not be applied to the pressure.

⇝ For the velocity and (if necessary) the turbulent variables, the values at the wall are calculated from theoretical profiles. In the case of a moving wall, the three components of the slipping velocity are given by (RCODCL(IFAC,IU(IPHAS),1), RCODCL(IFAC,IV(IPHAS),1), and RCODCL(IFAC,IW(IPHAS),1)).
WARNING: the wall moving velocity must be in the boundary face plane. By security, the code uses only the projection of this velocity on the face. As a consequence, if the velocity specified by the user is not in the face plane, the wall moving velocity really taken into account will be different.

⇝ For the other scalars, the condition ICODCL=5 is similar to ICODCL=1, but with a wall exchange coefficient calculated from a theoretical law. The values of RCODCL(IFAC,IVAR,1) and RCODCL(IFAC,IVAR,2) must therefore be specified: see [11].

- If ICODCL(IFAC,IVAR)=9: free outlet condition for the velocity. This condition can only be applied to the velocity components.
  If the mass flow at the face is going out, this condition is equivalent to a zero flow condition.
  If the mass flow at the face is coming in, the value zero is imposed to the velocity at the face (but not to the mass flow).
  RCODCL is not used.

- If ICODCL(IFAC,IVAR)=10: free outlet condition for the other variables. This condition can be applied to every variable apart from the velocity components and the pressure.
  If the mass flow at the face is going out, this condition is equivalent to a zero flow condition.
  If the mass flow at the face is coming in, this condition is equivalent to a Dirichlet condition. The array RCODCL(IFAC,IVAR,1) must therefore be completed in order to set the value of this Dirichlet.

NOTE
• A standard ISOR09 outlet face amounts to a Dirichlet condition (ICODCL=1) for the pressure, a free outlet condition (ICODCL=9) for the velocity and a zero flow condition (ICODCL=3) for the other variables.
• A standard ISOR10 outlet face amounts to a Dirichlet condition (ICODCL=1) for the pressure, a free outlet condition (ICODCL=9) for the velocity and a free outlet condition (ICODCL=10) for the other variables.

4.4.3 Checking of the boundary conditions

The code checks itself the main compatibilities between the boundary conditions. In particular, the following rules must be respected:
• On each face, the three components of the velocity must belong to the same type. The same must be true for the different components of the R_{ij} tensor.
• If the boundary conditions for the velocity belong to the "slipping" type (ICODCL=4), the conditions for R_{ij} must belong to the "symmetry" type (ICODCL=4), and vice versa.
• If the boundary conditions for the velocity belong to the "friction" type (ICODCL=5), the conditions for the turbulent variables must belong to the "friction" type, too.
• If the boundary condition for a scalar belongs to the "friction" type, the boundary condition for the velocity must belong to the "friction" type, too.

4.4.4 Sorting of the boundary faces

In the code, it may be necessary to have access to all the boundary faces of a given type. In order to ease this kind of search, an array of sorted faces is automatically completed (and updated at every time step) for each phase IPHAS: ITRIFB(NFABOR,IPHAS).
IFAC=ITRIFB(n,IPHAS) is the number of the n^{th} face of type 1.
IFAC=ITRIFB(n+N,IPHAS) is the number of the n^{th} face de type 2, if there are N faces of type 1.
... etc.

Two auxiliary arrays of size NTYPMX are also defined.
IDEBTY(ITYP,IPHAS) is the number of the first box corresponding to the faces of type ITYP in the array ITRIFB.
IFINTY(ITYP,IPHAS) is the number of the last box corresponding to the faces of type ITYP in the array ITRIFB.

Therefore, a number IFAC0 between IDEBTY(ITYP,IPHAS) and IFINTY(ITYP,IPHAS) corresponds to each face of type ITYP=ITYPFB(IFAC,IPHAS), so that IFAC=ITRIFB(IFAC0,IPHAS).

If there is no face of type ITYP, the code imposes
IFINTY(ITYP,IPHAS)=IDEBTY(ITYP,IPHAS)-1,
which allows to bypass, for all the missing ITYP, the loops like
`DO II=IDEBTY(ITYP,IPHAS),IFINTY(ITYP,IPHAS)`.

The values of all these indicators are displayed in the beginning of the code execution listing.

4.5 Management of the boundary conditions with LES: `usvort`

This subroutine allows to generate the non-stationary inlet boundary conditions for the LES by the vortex method. The method is based on the generation of vortices in the inlet 2D inlet plane with help from the pre-defined functions. The fluctuation normal to the inlet plane is generated by a Langevin equation. It is in the subroutine `usvort` where the parametres of this method of given.

subroutine called for each time step

To allow the application of the vortex method, an indicator must be informed of the method in the user subroutine `usini1`(ivrtex=1)

The subroutine `usvort` contains 3 seperate parts:

- The 1st part defines the number of inlets concerned with the vortex method(NNENTT) and them number of vortex for each inlet (NVORT), where IENT represents the number of inlets.

- The 2nd part (IAPPEL=1) defines the boundary faces at which the vortex method is applicable. The IREPVO array is informed by IENT which defines the number of inlets concerned with the vortex (essentially, the vortex method can be applied with many independant inlets).

- The 3rd section defines the main parameters of the method at each inlet. With the complexity of any given geometry, 4 cases are distinguished (the first 3 use the data file FIDCAT and in the final case only 1 initial velocity and energy are imposed.):

  * ICAS=1, For the outlet of a rectangluar pipe; 1 boundary condition is defined for each side of the rectangle takin ginto account their interaction with the vortex.
  * ICAS=2, For the outllet of a circular pipe; the entry face is considered as a wall (as far as interaction with the vortex is concerned)
  * ICAS=3, For inlets of any geometry; no boundary conditions are defined at the inlet face (i.e no specific treatment on the interation between the vortex and the boundary)
  * ICAS=4, similar to ICAS=3 except the data file is not used (FIDCAT); the outflow parameters are estimated by the code from the global data (initial velocity, level of turbulence and dissipation), information which is supplied by the user.

  When the geometry allows, cases 1 and 2 are used. Case 4 is only used if it is not possible to use the other 3.

  In the first 3 cases, the 2 base vectors in the plane of each inlet must be defined (vectors DIR1 and DIR2). The 3rd vector is automatically calculated by the code, defined as a product of DIR1 and DIR2. DIR1 and DIR2 must be chosen impreitavely to give (CEN, DIR1, DIR2) an orthoganol reference of the inlet plane and so DIR3 is orientated in the entry domain.If ICAS=2, the position CEN has to be the center of gravity of the rectangle or disc.

  The reference points (CEN, DIR1, DIR2, DIR3) wihch define the values of the variable in the FIDCAT file.
  In the case where ICAS=4, the vectors DIR1 and DIR2 are generated by the code.

If ICAS=1, The boundary condtions at the rectangle's edges must be defined. They are defined in the array ICLVOR. ICLVOR(II,IENT) represents the standard boundary conditions at the edge II($1 \leqslant II \leqslant 4$) of the inlet IENT. The code for the boundary conditions is as follows:

* ICLVOR=1 for a wall
* ICLVOR=2 for symmetry
* ICLVOR=3 for the periodicity of of transfer (the face corresponding to periodicity will automatically be taken as 3)

The 4 edges are numbered relative to the directions DIR1 and DIR2 as shown in figue 2:

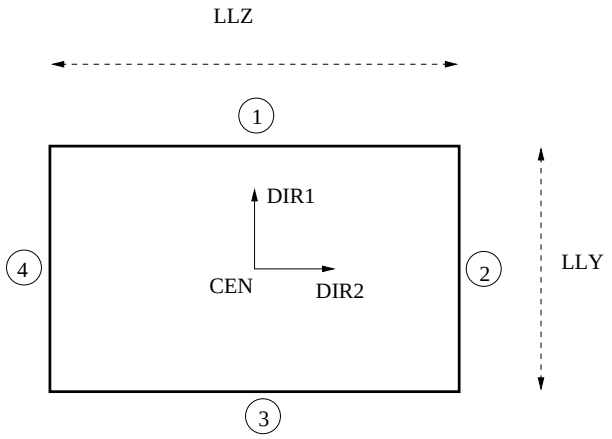

Figure 2: Numbering of the edges of a rectangular inlet(ICAS=1) treated by the vortex method

If ICAS=1, the user must define LLX and LLY which give the lengths of the rectangular pipe in the directions DIR1 and dir2.
If ICAS=2, LLD represents the diameter of the circular pipe. If ICAS=4, UDEBIT,KDEBIT and EDEBIT are defined for each inlet, these give respectively, initial speed, turbulent energy level and the dissipation level. These can be used to obtain their magnitude using the correlations in the user routine `usclim` for fully developed flow in a pipe.

The parameter not case dependant are defined as follows:

* ITMPL represents the indicator of the advancement in time of the vortex. If ITMPLI=1, the vortex will be regenerated after a fixed time of TMPLIM second (defined as ITMPLI=1). If ITMPLI=2, following hte data indicated in FIDCAT file, the vortex will have a variable life span equal to $5C_\mu \frac{k^{\frac{3}{2}}}{\varepsilon U}$, where $C_\mu = 0,09$ and k, ε and U represent respectively, turbulent energy, turbulent dissipation and the convective velocity in the direction normal to the inlet plane.
* XSIGMA represents the support functions used in the vortex method. They are representative of the eddy sizes entered in the vortex method. ISIGMA is used to define their size: if ISIGMA=1,nction with the co-ordinates XDAT and YDAT (given in the FIDCAT file). Note that using an indicator III to accelerate the calculations XSIGMA will be constant across the inlet face and is defined in `usvort`, if ISIGMA=2, nction with the co-ordinates XDAT and YDAT (given in the FIDCAT file). Note that using an indicator III to accelerate the calculationsXSIGMA will be variable and equal to the mixing length of the standard $k-\varepsilon$ model ($C_\mu{}^{\frac{3}{4}} \frac{k^{\frac{3}{2}}}{\varepsilon}$), if ISIGMA=3, XSIGMA will be equal to the maximum of L_t et L_K where L_t and L_K are the $\frac{\partial U}{\partial y}$ $\frac{\partial U}{\partial y}$ Taylor and Kolmogrov co-efficients ($L_T = (5\nu \frac{k}{\varepsilon})^{\frac{1}{2}}$, $L_K = 200(\frac{\nu^3}{\varepsilon})^{\frac{1}{4}}$).

* IDELPA gives the vortex displacement method in the 2D inlet plane (the vortex method is a langrangian method in which the eddy centers are replaced by a set velocity). If IDELPA=1, the velocity displacement referred to by UD which is the vortex following a random sampling (a sample number r, is taken for each vortex, at each time step and for each direction and the center of the vortex is replaced by the 2 principle directions, $r\mathrm{UD}\Delta t$ where Δt is the time step of the calcualtion). If IDEPLA=2, the vortex will be convected by itself (with the speed given by the time step before the vortex method)

A data file, FIDCAT, must be defined in the cases of ICAS=1,2,3, for each inlet. The data file must contain the following data in order (x, y, U, $\frac{\partial U}{\partial y}$, k, ε). The number of lines of the file is given by the interger NDAT. x and y are the co-ordinates in the inlet plane defined by the vectors DIR1 and DIR2. U, k and ε are respectively, the average speed normal to the inlet, the turbulent energy and the turbulent dissipation. $\frac{\partial U}{\partial y}$ is the derivative in the direction normal to the inlet boundary in the cases , ICAS=1, ICAS=2. Where ICAS=3 and ICAS=4 this variable is not applied (it is given the value 0)so the Langevin equations, used to generate fluctuations normal to the inlet plane, is de-activated (the flucutations normal to the inlet is 0 on both these cases). Note that the application of many different test of the Langevin equation doesn't have a notable influence on the results and that, by contrast it simply increases the computing time per iteration and so it decreases the random sampling which slows down the pressure solver. The interpolation used in the vortex method is defined by the function PHIDAT. An example is given at the end of `usvort` where the user can define the interpolation required. In the PHIDAT function, XX and YY are the co-ordinates by which the valu e of PHIDAT is calculated. XDAT and YDAT are the co-ordinates in the FIDCAT file. VARDAT is the value of the PHIDAT function with the co-ordinates XDAT and YDAT (given in the FIDCAT file). Note that using an indicator III accelerateas the calculations(the user need not modify or delete). The user must also define the parameter ISUIVO wich indicates if the vortex were started at 0 or if the file must be re-read (FICMVO).

WARNING

- Be sure that the FIDCAT file and the interpolation in the user function PHIDAT are compatible (in particular that all the entry region is covered by FIDCAT)
- If the user wants to use a 1D profile in the DIR2 direction, set x =0 in the FIDCAT file and define the interpolation in PHIDAT.

4.6 Management of the variable physical properties: `usphyv`

Subroutine called every time step.

If necessary, all the variation laws related to the fluid physical parameters (density, viscosity, thermal diffusivity ...) are written in this subroutine.

The validity of the variation laws must be checked, particularly when non-linear laws are defined (for instance, a third-degree polynomial law may produce negative density values).

WARNING

- If one wishes to impose a density or viscosity variable in `usphyv`, it can be done either in the interface or in `usini1`(IROVAR(IPHAS)=1, IVIVAR(IPHAS)=1).
- In order to impose a physical property (ρ, μ, λ, C_p)[25] a reference value must be inputted to the interface or in `usini1`(in particular for ρ, the pressure will contain 1 part as $\rho_0 gz$)

[25] except for some specific physics

- By default, the C_p coefficient of the phase IPHAS and the diffusivity of the scalars ISCAL (λ/C_p for the temperature) are considered as constant in time and uniform in space, with the values CP0(IPHAS) and VISLS0(ISCAL) specified in the interface or in `usini1`.
  To give a variable value to C_p, the user must specify it in the interface or give the value 1 to ICP(IPHAS) in `usini1`, and complete for each cell IEL the array PROPCE(IEL,IPCCP) in `usphyv`. Completing the array PROPCE(IEL,IPCCP) while ICP(IPHAS)=0 induces array overwriting problems and produces wrong results.

- In the same way, to have variable diffusivities for the scalars ISCAL, the user must specify it in the interface or give the value 1 to IVISLS(ISCAL) in `usini1`, and complete for each cell IEL the array PROPCE(IEL,IPCVSL) in `usphyv`. Completing PROPCE(IEL,IPCVSL) while IVISLS(ISCAL)=0 induces memory overwriting problems and produces wrong results.

  Example: If the scalars 1 and 3 have a constant and uniform viscosity, and if the scalars 2 and 4 have a variable viscosity, the following values must be imposed in `usini1`:
  IVISLS(1)=0, IVISLS(2)=1, IVISLS(3)=0 and IVISLS(4)=1.
  The indicators IVISLS(2) and IVISLS(4) are then modified automatically by the code in order to reflect the rank corresponding to the diffusivity of each scalar in the list of physical properties[26]. The arrays PROPCE(IEL,IPCVSL) in `usphyv` must then be completed with IPCVSL=IPPROC(IVISLS(2)) and IPCVSL=IPPROC(IVISLS(4)).

  Note: The indicators IVISLS must not be completed in the case of user scalars representing the average of the square of the fluctuations of another scalar, because the diffusivity of a user scalar JJ representing the average of the square of the fluctuations of a user scalar KK comes directly from the diffusivity of this last scalar. In particular, the diffusivity of the scalar JJ is variable if the diffusivity of KK is variable.

4.7 Non-standard initialisation of the variables: `usiniv`

Subroutine only called during calculation initialisation.

At the calculation beginning, the variables are initialised automatically by the code. Velocities and scalars are set to the value 0 (or SCAMAX or SCAMIN if 0 is outside the acceptable scalar variation range), and the turbulent variables are estimated from UREF and ALMAX.
For k in $k-\varepsilon$, $R_{ij}-\varepsilon$, v2f or $k-\omega$ model:
`RTP(IEL,IKIPH) = 1.5D0*(0.02D0*UREF(IPHAS))**2` (in $R_{ij}-\varepsilon$, $R_{ij}=\frac{2}{3}k\delta_{ij}$)
For ε in $k-\varepsilon$, $R_{ij}-\varepsilon$ or v2f model:
`RTP(IEL,IEIPH) = RTP(IEL,IKIPH)**1.5D0*CMU/ALMAX(IPHAS)`
For ω in $k-\omega$ model:
`RTP(IEL,IOMGIP) = RTP(IEL,IKIPH)**0.5D0/ALMAX(IPHAS)`
For φ and $\overline{f}$ in v2f model:
`RTP(IEL,IPHIPH) = 2.D0/3.D0`
`RTP(IEL,IFBIPH) = 0.D0`

The subroutine `usiniv` allows if necessary to initialise some variables at values closer to their estimated final values, in order to obtain a faster convergence.

This subroutine allows also to make non-standard initialisation of physical parameters (density, viscosity, ...), to impose a local value of the time step, or to modify some parameters (time step, variable specific heat, ...) in the case of a calculation restart.

NOTE: VALUE OF THE TIME STEP

[26] they are no longer worth 1 but stay positive so that IVISLS>0 is synonymous with variable property

- In the case of a calculation with constant and uniform time step (IDTVAR=0), the value of the time step is DTREF, given in the parametric file of the interface or `usini1`, the calculation being whether a restart (ISUITE=1) or not (ISUITE=0).

- In the case of a calculation with non-constant time step (IDTVAR=1 or 2) which is not a calculation restart (ISUITE=0), the value of DTREF given in the parametric file of the interface or in `usini1` is used to initialise the time step.

- In the case of a calculation with non-constant time step (IDTVAR=1 or 2) which is a restart (ISUITE=1) of a calculation whose time step type was different (for instance, restart using a variable time step of a calculation run using a constant time step), the value of DTREF given in the parametric file of the interface or in `usini1` is used to initialise the time step.

- In the case of a calculation with non-constant time step (IDTVAR=1 or 2) which is a restart (ISUITE=1) of a calculation whose time step type was the same (for instance, restart with IDTVAR=1 of a calculation run with IDTVAR=1), the time step is read from the restart file and the value of DTREF given in the parametric file of the interface or in `usini1` is not used.

It follows that for a calculation with non-constant time step (IDTVAR=1 or 2) which is a restart (ISUITE=1) of a calculation in which IDTVAR had the same value, DTREF does not allow to modify the time step. The user subroutine `usiniv` allows to modify the array DT which contains the value of the time step read from the restart file (array whose size is NCELET, defined at the cell centers whatever the chosen time step type).

WARNING: to initialise the variables in the framework of a specific physics module (NSCAPP.GT.0) *one of the subroutines* ***`usebui`****,* ***`usd3pi`****,* ***`uslwci`*** *or* ***`uscpiv`*** *should be used instead of* ***`usiniv`*** *(depending on the activated module).*

4.8 Non-standard management of the chronological record files: `ushist`

Subroutine called every time step

The interface and the subroutine `usini1` allow to manage the "automatic" chronological record files in an autonomous way: position of the probes, printing frequency and concerned variables. The results are written in a different file for each variable. These files are written in *xmgrace or* gnuplot format and contain the profiles corresponding to every probe. This type of output format may not be well adapted if, for instance, the number of probes is too high. The subroutine `ushist` allows then to personalise the output format of the chronological record files. The version given as example in the directory works as follows:

- Positionning of the probes (only at the first passage): the index II varies between 1 and the number of probes. The coordinates XX, YY and ZZ of each probe are given. The subroutine `findpt` gives then the number ICAPT(II) of the cell center which is the closest to the defined probe.

- Opening of the writing files (only at the first passage): in the version given as example, the program opens a different file for all the NVAR variables. FICUSH(J) contains the name of the J^{th} file and IMPUSH(J) its unit number (IMPUSH is initialised by default so that the user has at his disposal specific unit numbers and does not run the risk to overwrite an already open file).

- Writing in the files: in the version given as example, the program writes the time step number, the physical time step (based on the standard time step in the case of a variable time step) and the value of the selected variable at the different probes.

- Closing of the files (only at the last time step).

WARNING: The use of `ushist` *neither erases nor replaces the parameters given in the interface or in* `usini1`*. Therefore, in the case of the use of* `ushist`*, and to avoid the creation of useless files, the user should set* NCAPT=0 *in the interface or in* `usini1` *to deactivate the automatical production of chronological records.*
In addition, ***`ushist`*** generates supplementary result files. The user shoud remember to add in the launch script the necessary command to copy them in the directory `RESU` at the end of the calculation. The interface allows the specification of the name of the copied user results files. For the calculations without interface, the variable must be inputted in FICHIERS_RESULTATS_UTILISATEUR in the launch script.

4.9 User source terms in Navier-Stokes: `ustsns`

Subroutine called every time step

This subroutine is used to add user source terms to the Navier-Stokes equations. For each phase IPHAS, it is called three times every time step, once for each velocity component (IVAR is successively worth IU(IPHAS), IV(IPHAS) and IW(IPHAS)). At each passage, the user must complete if necessary the arrays CRVIMP and CRVEXP expressing respectively the implicit and explicit part of the source term. If no other source terms apart from IVAR=IU(IPHAS)for example, are require d, CRVIMP and CRVEXP must be read over and their 2 other components, IVAR=IV(IHPAS) and IVAR=IW(IPHAS) must be cancelled.

WARNING: The decomposition of the soure terms of CVRIMP/CRVEXP is different to that of the code ESTET: be careful of reflex working

Let us assume that the user source terms modify the equation of a variable φ in the following way:

$$\rho\frac{\partial\varphi}{\partial t}+\ldots=\ldots+S_{impl}\times\varphi+S_{expl}$$

φ is here a velocity component, but the examples are also valid for a turbulent variable (k, ε, R_{ij}, ω, φ or $\overline{f}$) and for a scalar (or for the average of the square of the fluctuations of a scalar), because the syntax of the subroutines `ustske`, `ustsri`, `ustsv2`, `ustskw` and `ustssc` is similar.

In finite volume formulation, the solved system is then modified as follows:

$$\left(\frac{\rho_i\Omega_i}{\Delta t_i}-\Omega_iS_{impl,i}\right)\left(\varphi_i^{(n+1)}-\varphi_i^{(n)}\right)+\ldots=\ldots+\Omega_iS_{impl,i}\varphi_i^{(n)}+\Omega_iS_{expl,i}$$

The user needs therefore to provide the following values:
$\text{CRVIMP}_i=\Omega_iS_{impl,i}$
$\text{CRVEXP}_i=\Omega_iS_{expl,i}$

In practice, it is essential that the term $\left(\frac{\rho_i\Omega_i}{\Delta t_i}-\Omega_iS_{impl,i}\right)$ is positive. To ensure this property, the equation really taken into account by the code is the following:

$$\left(\frac{\rho_i\Omega_i}{\Delta t_i}-\text{Min}(\Omega_iS_{impl,i};0)\right)\left(\varphi_i^{(n+1)}-\varphi_i^{(n)}\right)+\ldots=\ldots+\Omega_iS_{impl,i}\varphi_i^{(n)}+\Omega_iS_{expl,i}$$

To make the "implicitation" effective, the source term decomposition between implicit and explicit parts will be done by the user who must make sure $\text{CRVIMP}_i=\Omega_iS_{impl,i}$ is always negative (otherwise the solved equation remains right, but there is no "implicitation").

WARNING: When the second-order in time with extrapolation of the source terms[27] *is activated, it is no longer possible to test the sign of $S_{impl,i}$, because of coherence reasons (for more details, the user may refer to the theoretical and computer documentation [11] of the subroutine texttttpreduv). The user must therefore make sure it is always positive.*

[27] indicator `ISNO2T` for the velocity, `ISTO2T` for the turbulence and `ISSO2T` for the scalars

Particular case of a linearised source term

In some cases, the added source term is not linear, but the user may want to linearise it using a first-order Taylor development, in order to make it partially implicit.
Let us consider an equation of the type:

$$\rho\frac{\partial\varphi}{\partial t} = F(\varphi)$$

We want to make it implicit using the following method:

$$\begin{aligned}\frac{\rho_i\Omega_i}{\Delta t}\left(\varphi_i^{(n+1)}-\varphi_i^{(n)}\right) &= \Omega_i\left[F(\varphi_i^{(n)})+\left(\varphi_i^{(n+1)}-\varphi_i^{(n)}\right)\frac{dF}{d\varphi}(\varphi_i^{(n)})\right]\\ &= \Omega_i\frac{dF}{d\varphi}(\varphi_i^{(n)})\times\varphi_i^{(n+1)}+\Omega_i\left[F(\varphi_i^{(n)})-\frac{dF}{d\varphi}(\varphi_i^{(n)})\times\varphi_i^{(n)}\right]\end{aligned}$$

The user must therefore specify:
$\text{CRVIMP}_i = \Omega_i\frac{dF}{d\varphi}(\varphi_i^{(n)})$
$\text{CRVEXP}_i = \Omega_i\left[F(\varphi_i^{(n)})-\frac{dF}{d\varphi}(\varphi_i^{(n)})\times\varphi_i^{(n)}\right]$

Example:
If the equation is $\rho\frac{\partial\varphi}{\partial t} = -K\varphi^2$, the user must set:
$\text{CRVIMP}_i = -2K\Omega_i\varphi_i^{(n)}$
$\text{CRVEXP}_i = K\Omega_i[\varphi_i^{(n)}]^2$

4.10 User source terms for k and ε: `ustske`

Subroutine called every time step, in $k-\varepsilon$ and in v2f.

This subroutine is used to add source terms to the transport equations related to the turbulent kinetics energy k and to the turbulent dissipation ε (for each phase IPHAS). This subroutine is called every time step, once for each phase (the treatment of the two variables k and ε is made simultaneously). The user is expected to provide the arrays CRKIMP and CRKEXP for k and CREIMP and CREEXP for ε. These arrays are similar to the arrays CRVIMP and CRVEXP given for the velocity in the user subroutine `ustsns`. The way of making implicit the resulting source terms is the same as the one presented in `ustsns`.For φ and $\bar{f}$ in v2f, see `ustsv2`, §4.12.

4.11 User source terms for R_{ij} and ε: `ustsri`

Subroutine called every time step, in $R_{ij}-\varepsilon$.

This subroutine is used to add source terms to the transport equations related to the Reynolds stress variables R_{ij} and to the turbulent dissipation ε (for each phase IPHAS). This subroutine is called 7 times every time step and for each phase (once for each Reynolds stress component and once for the dissipation). The user must provide the arrays CRVIMP and CRVEXP for the variable IVAR (referring successively to IR11(IPHAS), IR22(IPHAS), IR33(IPHAS), IR12(IPHAS), IR13(IPHAS), IR23(IPHAS) and IEP(IPHAS)). These arrays are similar to the arrays CRVIMP and CRVEXP given for the velocity in the user subroutine `ustsns`. The way of making implicit the resulting source terms is the same as that presented in `ustsns`.

4.12 User source terms for φ and $\overline{f}$: `ustsv2`

Subroutine called every time step, in v2f.

This subroutine is used to add source terms to the transport equations related to the variables φ and $\overline{f}$ of the v2f φ-model (for each phase IPHAS). This subroutine is called twice every time step and for each phase (once for φ and once for $\overline{f}$). The user is expected to provide the arrays CRVIMP and CRVEXP for IVAR referring successively to IPHI(IPHAS) and IFB(IPHAS). Concerning φ, these arrays are similar to the arrays CRVIMP and CRVEXP given for the velocity in the user subroutine `ustsns`. Concerning $\overline{f}$, the equation is slightly different:

$$L^2 div(\underline{\text{grad}}\ (\overline{f})) = \overline{f} + \ldots + S_{impl} \times \overline{f} + S_{expl}$$

In finite volume formulation, the solved system is written:

$$\int_{\partial\Omega_i} \underline{\text{grad}}\ (\overline{f})^{(n+1)} dS = \frac{1}{L_i^2}\left(\Omega_i \overline{f}_i^{(n+1)} + \ldots + \Omega_i S_{impl,i} \overline{f}_i^{(n+1)} + \Omega_i S_{expl,i}\right)$$

The user must then specify:
$\text{CRVIMP}_i = \Omega_i S_{impl,i}$
$\text{CRVEXP}_i = \Omega_i S_{expl,i}$

The way of making implicit the resulting source terms is the same as the one presented in `ustsns`.

4.13 User source terms for k and ω: `ustskw`

Subroutine called every time step, in $k-\omega$.

This subroutine is used to add source terms to the transport equations related to the turbulent kinetics energy k and to the specific dissipation rate ω (for each phase IPHAS). This subroutine is called every time step, once for each phase (the treatment of the two variables k and ω is made simultaneously).The user is expected to provide the arrays CRKIMP and CRKEXP for the variable k the arrays CRWIMP and CRWEXP for the variable ω. These arrays are similar to the arrays CRVIMP and CRVEXP given for the velocity in the user subroutine `ustsns`. The way of making implicit the resulting source terms is the same as the one presented in `ustsns`.

4.14 User source terms for the user scalars: `ustssc`

Subroutine called every time step.

This subroutine is used to add source terms to the transport equations related to the user scalars (passive or not, average of the square of the fluctuations of a scalar ...). In the same way as `ustsns`, this subroutine is called every time step, once for each user scalar. The user needs to provide the arrays CRVIMP and CRVEXP related to each scalar. CVIMP and CRVEXP must be set to 0 for the scalars on which it is not wished for the user source term term to be applied (the arrays are initially at 0 at each inlet in the subroutine.)

4.15 Management of the pressure drops: `uskpdc`

Subroutine called every time step.

This subroutine is called three times every time step and for each phase IPHAS.

The tensor representing the pressure drops is supposed to be symmetric and positive.

- During the first call, all the cells are checked to know the number of cells in which a pressure drop is present for the phase IPHAS. This number is called NCEPDP in `uskpdc` (and corresponds to

NCEPDC(IPHAS)). It is used to lay out the arrays related to the pressure drops. If there is no pressure drop, NCEPDP must be equal to zero (it is the default value, and the rest of the subroutine is then useless).

- During the second call, all the cells are checked again to complete the array ICEPDP whose size is NCEPDP. ICEPDC(IELPDC) is the number of the IELPDC$^{\text{th}}$ cell containing pressure drops (for the current phase). It is specified if the tensor of pressure drops will be diagonal (3 elements) or not (6 elements), by means of the variable NCKPDP=NCKPDC(IPHAS), which is worth 3 or 6.

- During the third call, all the cells containing pressure drops (for the current phase) are checked in order to complete the array containing the components of the tensor of pressure drops CKUPDC(NCEPDP,NCKPDP). This array is so that the equation related to the velocity may be written:

$$\rho \frac{\partial}{\partial t}\underline{u} = \ldots - \rho \underline{\underline{K}}_{pdc} \cdot \underline{u}$$

  The tensor components are given in the following order (in the general reference frame):: K11, K22, K33 or K11, K22, K33, K12, K13, K23 (depending on wether NCKPDP is worth 3 or 6).

The three calls are made every time step, so that variable pressure drop zones or values may be treated.

4.16 Management of the mass sources: `ustsma`

Subroutine called every time step.

This subroutine is used to add a density source term in some cells of the domain. The mass conservation equation is then modified as follows:

$$\frac{\partial \rho}{\partial t} + div(\rho \underline{u}) = \Gamma$$

Γ is the mass source term expressed in $kg.m^{-3}.s^{-1}$.

The presence of a mass source term modifies the evolution equation of the other variables, too. Let φ be a any solved variable apart from the pressure (velocity component, turbulent energy, dissipation, scalar ...). Its evolution equation becomes:

$$\rho \frac{\partial \varphi}{\partial t} + \ldots = \ldots + \Gamma(\varphi_i - \varphi)$$

φ_i is the value of φ associated with the mass entering or leaving the domain. After discretisation, the equation may be written:

$$\rho \frac{\varphi^{(n+1)} - \varphi^{(n)}}{\Delta t} + \ldots = \ldots + \Gamma(\varphi_i - \varphi^{(n+1)})$$

For each variable φ, there are two possibilities:

- We can consider that the mass is added (or removed) with the ambient value of φ. In this case $\varphi_i = \varphi^{(n+1)}$ and the equation of φ is not modified.

- Or we can consider that the mass is added with an imposed value φ_i (this solution is physically correct only when the mass is effectively added, $\Gamma > 0$).

This subroutine is called three times every time step (for each phase).

- During the first call, all the cells are checked to know the number of cells containing a mass source term for the current phase IPHAS. This number is called NCESMP in `ustsma` (and corresponds to NCETSM(IPHAS)). It is used to lay out the arrays related to the mass sources. If there is no mass source, NCESMP must be equal to zero (it is the default value, and the rest of the subroutine is then useless).
- During the second call, all the cells are checked again to complete the array ICETSM whose dimension is NCESMP. ICETSM(IELTSM) is the number of the IELTSM$^{\text{th}}$ cell containing a mass source (for the current phase).
- During the third call, all the cells containing mass sources are checked in order to complete the arrays ITYPSM(NCESMP,NVAR) and SMACEL(NCESMP,NVAR):
  - ITYPSM(IELTSM,IVAR) is the flow type associated with the variable IVAR in the IELSTM$^{\text{th}}$ cell containing a mass source.
    ITYPSM=0: $\varphi_i = \varphi^{(n+1)}$ condition
    ITYPSM=1: imposed φ_i condition
    ITYPSM is not used for IVAR=IPR(IPHAS)
  - SMACEL(IELTSM,IPR(IPHAS)) is the value of the mass source term Γ, in $kg.m^{-3}.s^{-1}$.
  - SMACEL(IELTSM,IVAR), for IVAR different from IPR(IPHAS), is the value of φ_i for the variable IVAR in the IELSTM$^{\text{th}}$ cell containing a mass source.

  NOTES
  • If ITYPSM(IELTSM,IVAR)=0, SMACEL(IELTSM,IVAR) is not used.
  • If Γ=SMACEL(IELTSM,IPR(IPHAS))<0, mass is removed from the system, and *Code_Saturne* considers automatically a $\varphi_i = \varphi^{(n+1)}$ condition, whatever the values given to ITYPSM(IELTSM,IVAR) and SMACEL(IELTSM,IVAR) (the extraction of a variable is done at ambient value).

The three calls are made every time step, so that variable mass source zones or values may be treated.

For the variance, do not take into account the scalar φ_i in the envronment where $\varphi \neq \varphi_i$ generates a variance source.

4.17 Thermal module in a 1D wall

subroutine called at every time step

This subroutine takes into account the affected thermal inertia by a wall. Some boundary faces are treated as a solid wall with a given thickness, on which the code resolves an undimensional equation for the heat conduction. The coupling between the 1D module and the fluid works in a similar way to the coupling with the SYRTHES. In construction, the user is not able to account for the heat transfer between different parts of the wall. A physical analysis of each problem, case by case is required to evaluate the relevance of its usage by way of a report of the simple conditions (temperature, zero flow) or a coupling with SYRTHES.

The use of this code requires that theres is only 1 phase (NPHAS=1) and that the thermal scalar is defined as (ISCALT> 0).

WARNING: The 1D thermal module is developped assuming the thermal scalar as a temperature. If the thermal scalar is an enthalpy, the code calls the subroutine **`usthht`** *for each transfer of information between the fluid and the wall in order to convert the enthalpy to temperature and vice-versa. This function has not been tested and is firmly discouraged . If the thermal variable is the total (compressible) energy, the thermal module will not work.*

This procedure is called twice,on initialisation and again at each time step.

- The 1st call (initialisation) all the boundary faces that will be treated as a coupled wall are marked out. This figure is written noted as NFKPT1D. It applies dimension to the arrays in the thermal module. NFKPT1D will be at 0 if there are no coupled faces (it is in fact the default value, the remainer of the subroutine is not used in this case). The parameter ISUIT1 also need to be defined, this indicates if the temperature of the wall must be initialised or written in the file (stored in the variable FILMT1).

- The 2nd call (initialisation)again concern the wall faces, it completes the IFPT1D array of dimension NFPT1D. IFPT1D(IFBT1D)is the number IFBT1D$^{\text{th}}$ boundary faces coupled with the thermal module of a 1D wall. The discretional parameters are then completed for a pseudo wall accosiated to each face

  - NPPT1D(NFPT1D): number of cells in the 1D mesh associated to the pseudo wall.
  - EPPT1D(NFPT1D): thickness of the pseudo wall.
  - RGPT1D(NFPT1D): geometery of the pseudo wall mesh (refined as a fluid if RGT1D is smaller than 1)
  - TPPT1D(NFPT1D): initialisation temperature of the wall (uniform in thckness). In the course of the calculation, the array stores the temperature of the solid at the fluid/solid interface.

  Other than for re-reading a file (FICMT1), TPPT1D is not used. NPPT1D, IFPT1D, RGPT1D and EPPT1D are compared to data from the follow-up file and they must be identical.

  WARNING: The test in IFPT1D implicilty assumes that the array is completed in ascending order (i.e IFPT1D(II)>IFPT1D(JJ) if II>JJ. This will be the case if the coupled faces are defined starting from the unique loop on the boundary faces (as in the example). If this is not the case, contact the development team to short circuit the test.

- The 3rd call (at each time step) is for the confirmation that all the arrays involving physical parameter and external boundary conditions have been completed.

  - ICLT1D(NFPT1D):Typical boundary condition at the external (pseudo) wall: Dirichlet condition (ICLT1D=1) or flow condition (ICLT1D=3)
  - TEPT1D(NFPT1D): External temperature of the pseudo wall in the Dirichlet case.
  - HEPT1D(NFPT1D): External coefficient of transfer in the pseudo wall under Dirichlet conditions(en $W.m^{-2}.K^{\cdot}$).
  - FEPT1D(NFPT1D): External heat flow in the pseado wall under the flow conditions(en $W.m^{-2}$,negative value for energy entering the wall)
  - XLMT1D(NFPT1D): Conductivityλ of the wall uniform in thickness, (in $W.m^{-1}.K^{-1}$).
  - RCPT1D(NFPT1D): Volumetric heat capacity ρC_p of the wall uniform in thickness in $J.m^{-3}.K^{-1}$)
  - DTPT1D(NFPT1D): Physical time step ascociated with the solved 1D equation of the pseudo wall(which can be different from the time step in the calcualtion)

The 3rd call, done at each time step, allows the imposition of boundary conditions and physical values in time.

4.18 Modification of the turbulent viscosity: `usvist`

Subroutine called every time step.

This subroutine is used to modify the calculation of the turbulent viscosity of the phase IPHAS, *i.e.* μ_t in $kg.m^{-1}.s^{-1}$ (this piece of information, at the mesh cell centers, is conveyed by the variable PROPCE(IEL,IPCVST), with IPCVST = IPPROC(IVISCT(IPHAS))). The subroutine is called at

the beginning of every time step, after the calculation of the physical parameters of the flow and of the "conventional" value of μ_t corresponding to the chosen turbulence model (indicator ITURB(IPHAS)). *WARNING: The calculation of the turbulent viscosity being a particularly sensible stage, a wrong use of* `usvist` *may distort seriously the results.*

4.19 Modification of the friction velocity: `usruet`

Subroutine called every time step for every wall face.

This subroutine is used to modify the calculation of the friction velocity u_* (variable UET) for each phase. For more precisions concerning the friction velocity and the wall boundary conditions, the user may refer to the report [4] and to the theoretical and computer documentation [11] of the subroutine `clptur`. To access to this document from a workstation, use the command `info_cs noyau`.

The subroutine allows in particular to access to the value of y^+ at the wall.

4.20 Modification of the variable C of the dynamic LES model: `ussmag`

Subroutine called every time step in the case of LES with the dynamic model.

This subroutine is used to modify the calculation of the variable C of the LES sub-grid scale dynamic model.

Let us first remind that the LES approach introduces the notion of filtering between large eddies and small motions. The solved variables are said to be filtered in an "implicit" way. Sub-grid scale models ("dynamic" models) introduce in addition an explicit filtering.

The notations used for the definition of the variable C used in the dynamic models of *Code_Saturne* are specified below. These notations are the ones assumed in the document [2], to which the user may refer for more details.

The value of a filtered by the explicit filter (of width $\widetilde{\overline{\Delta}}$) is called $\widetilde{a}$ and the value of a filtered by the implicit filter (of width $\overline{\Delta}$) is called $\overline{a}$. We define:

$$\begin{array}{ll} \overline{S}_{ij} = \frac{1}{2}(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}) & ||\overline{S}|| = \sqrt{2\overline{S}_{ij}\overline{S}_{ij}} \\ \alpha_{ij} = -2\widetilde{\overline{\Delta}}^2 ||\widetilde{\overline{S}}||\widetilde{\overline{S}}_{ij} & \beta_{ij} = -2\overline{\Delta}^2||\overline{S}||\overline{S}_{ij} \\ L_{ij} = \widetilde{\overline{u}_i\overline{u}_j} - \widetilde{\overline{u}}_i\widetilde{\overline{u}}_j & M_{ij} = \alpha_{ij} - \widetilde{\beta}_{ij} \end{array} \quad (1)$$

In the framework of LES, the total viscosity (molecular + sub-grid) in $kg.m^{-1}.s^{-1}$ may be written in *Code_Saturne*:

$$\begin{array}{lcll} \mu_{\text{total}} & = & \mu + \mu_{\text{sub-grid}} & \text{if } \mu_{\text{sub-grid}} > 0 \\ & = & \mu & \text{otherwise} \\ \text{with } \mu_{\text{sub-grid}} & = & \rho C \overline{\Delta}^2 ||\overline{S}|| & \end{array} \quad (2)$$

$\overline{\Delta}$ is the width of the implicit filter, defined at the cell Ω_i by
$\overline{\Delta} = XLESFL(IPHAS) * (ALES(IPHAS) * |\Omega_i|)^{BLES(IPHAS)}$.

In the case of the Smagorinsky model (ITURB(IPHAS)=40), C is a constant which is worth C_s^2. C_s^2 is the so-called Smagorinsky constant and is stored the variable $CSMAGO$.

In the case of the dynamic model (ITURB(IPHAS)=41), C is variable in time and in space. It is determined by $C = \dfrac{M_{ij}Lij}{M_{kl}M_{kl}}$.

In practice, in order to increase the stability, the code does not use the value of C obtained in each cell, but an average with the values obtained in the neighboring cells (this average uses the extended

neighborhood and corresponds to the explicit filter). By default, the value calculated by the code is

$$C = \frac{\widetilde{M_{ij}Lij}}{\widetilde{M_{kl}M_{kl}}}$$

The subroutine `ussmag` allows to modify this value. It is for example possible to calculate the local average after having calculated the ratio

$$C = \left[\frac{\widetilde{M_{ij}Lij}}{M_{kl}M_{kl}}\right]$$

WARNING: The subroutine `ussmag` *can be activated only when the dynamic model is used.*

4.21 Temperature-enthalpy and enthalpy-temperature conversions: `usthht`

Subroutine optionally called.

This subroutine is used to encapsulate a simple enthalpy-temperature conversion law and its inverse. This subroutine is called in `usray4`, user subroutine from the radiation module.

4.22 Modification of the mesh geometry: `usmodg`

Subroutine called only during the calculation initialisation.

This subroutine may be used to modify "manually" the mesh vertices coordinates, *i.e.* the array:

- XYZNOD(3,NNOD) (vertices coordinates)

WARNING: Caution must be exercised when using this subroutine along with periodicity. Indeed, the periodicity parameters are not updated accordingly, meaning that the periodicity may be unadapted after one changes the mesh vertices coordinates. It is particularly true when one rescales the mesh.

4.23 Management of the post-processing intermediary outputs: `usnpst`

Subroutine called every time step(even if the user hasn't moved it to the FORT directroy).

This subroutine is used to determine when post-processing outputs will be generated. By default, it tests if the current time step number (NTCABS) is a multiple of the chosen output frequency (NTCHR). If it is the case, the indicator IIPOST turns to 1, which triggers the writing of an intermediary output. If the frequency is given a negative value, the test is not done.

For instance, a user who wants to generate post-processing outputs (also called "chronological outputs") at the time step number 36 and around the physical time t=12 seconds may use the following test:

```
IIPOST = 0                                  No output by default.
IF (NTCABS.EQ.36) THEN                      If the current time step is the 36th,
   IIPOST=1                                   generate an output.
ENDIF                                       End of the test on the time step number.
IF (ABS(TTCABS-12.D0).LE.0.01D0) THEN       If the physical time is 12s +/- 0.01s,
   IIPOST=1                                   generate an output.
ENDIF                                       End of the test on the physical time.
```

In any case, a post-processing output is generated after the last time step, `usnpst` being used or not.

4.24 Definition of sections for outputs in the form of lists of faces: uslfac

Subroutine called at the calculation beginning.

This subroutine gives the possibility to define sections in the form of lists of NLFAC internal faces (LSTFAC) and NLFAB boundary faces (LSTFAB), in order to generate chronological outputs in *EnSight*, *MED* or *CGNS* format.

The given example proposes to define two sections (NBCOUP = 2). The first one is consituted of internal and boundary faces marked out by means of the coordinates of their centers. The second one is constituted of internal faces marked out by means of the color of their neighboring cells and of boundary faces marked out by means of their color.

It must be noticed that the lists of faces can not be modified during the calculation (they are set at the calculation beginning).

In order to ease the post-processing, a distinct name should be given to each section (COUPE =): this character string will be the name of the corresponding *EnSight* "part" and will be used in the eventual *MED* file.

The content of the character string CAS = will be used as a prefix in the name of the EnSight directory containing the post-processing files and in the eventual MED file. If several sections are requested and the user does not wish to post-process the data on each one at the same time step (see usvfac), it may be useful, in order to ease the post-processing, to specify a different value of CAS for each section (for instance CAS=''CAS_COUPE1'', CAS=''CAS_COUPE2''...), so that a distinct *EnSight* directory will be generated for each one. If CAS is not specified, the post-processing files are stored with the usual chronological post-processing files (it is recommended to always specify the value of the variable CAS).

The post-processing format is set by means of the variable FORMA = . By default, the *EnSight* format is generated. Outputs in the *MED* or *CGNS* formats may be also requested.

The values to post-process on the sections are precisely defined in the subroutine usvfac

4.25 Definition of the data to post-process on the sections: usvfac

Subroutine called every time step and for every section.

For the sections defined in uslfac, the subroutine usvfac is used to define the instants at which outputs will be generated and to specify which variables have to be post-processed. Basically, the communication for the current section is initialised by calling MSGDSC, which provides the section number, the time step number and the physical time. For this section, the arrays of values at internal (TRAFAI) and boundary faces (TRAFAB) are sent to the Preprocessor by the subroutine MSGVAC, as are the variable name (NAMEVR), the length of the character string which contains it (LNAME), the dimension of the variable (IDIMT=1 for a scalar and =3 for a vector) and the numbers of the section internal (NFAICP) and boundary (NFABCP) faces.

More precisely, the user must first define the pairs (section, time step) corresponding to expected post-processing outputs. This is the goal of the first part of the subroutine: an instruction RETURN is placed in the beginning of the subroutine according to the section number NUMCOU and the time step number NTCABS. It is important to note that the section outputs are independent from the other post-processing outputs. In particular, there is no automatically generated output after the last calculation time step (if an output after the last time step is wanted, this must then be specified).

For each section, the given example proposes then to define the variables to post-process. For instance, concerning the section number 1, the velocity, the pressure and the temperature at the boundary are generated. Concerning the section number 2, all the usually post-processed unknowns (according to NTCHR and ICHRVR) are generated.

4.26 Definition of post-processing and mesh zones: `usdpst`

Subroutine called at the calculation beginning..

This subroutine allows for the definition of surface or volume sections, in the form of lists of `NLFAC` internal faces (`LSTFAC`) and `NLFAB` boundary faces (`LSTFAB`), or of `NLCEL` cells (`LSTCEL`), in order to generate chronological outputs in *EnSight*, *MED* or *CGNS* format.

One or several "writers" can be associated with each visualization mesh, or "part" created. The arguments of the function `pstcwr` defining a "writer" are as follows:

- `NOMCAS`: basic name of the associated case.
  WARNING: depending on the chosen format, this name may be shortened (maximum number of characters: 32 for *MED*, 19 for *EnSight*) or modified automatically (whitespaces or forbidden characters will be replaced by '_')
- `NOMREP`: name of the output directory
- `NOMFMT`: choice of the output format:
  - → *EnSight Gold* (*EnSight* also accepted)
  - → *MED_fichier* (*MED* also accepted)
  - → *CGNS*
  - → *text* (readable with a text editor, mesh output, no variables output, for diagnosis purposes only).

  The options are not case-sensitive, so *ensight* or *cgns* are valid, too.
- `OPTFMT`: character string containing a list of options related to the format, separated by commas; for the *EnSight Gold* format, these options are:
  - → *binary* for a binary format version (by default)
  - → *text* for a text format version
  - → *discard_polygons* to prevent from exporting faces with more than four edges (which may not be recognized by some post-processing tools); such faces will therefore not appear in the post-processing mesh.
  - → *discard_polyhedra* to prevent from exporting elements which are neither tetrahedra, prisms, pyramids nor hexahedra (which may not be recognized by some post-processing tools); such elements will therefore not appear in the post-processing mesh.
  - → *divide_polygons* to divide faces with more than four edges into triangles, so that any post-processing tool can recognise them
  - → *divide_polyhedra* to divide elements which are neither tetrahedra, prisms, pyramids nor hexahedra into simpler elements (tetrahedra and pyramids), so that any post-processing tool can recognise them
  - → *split_tensor* to export the components of a tensor variable as a series of independent variables (a variable is recognised as a tensor if its dimension is 6 or 9); not implemented yet.
- `INDMOD`: indicates if the post-processing (i.e. visualization) meshes (or "parts") are:
  - → 0 fixed ("classic" case)
  - → 1 deformable (the vertex positions may vary over time)
  - → 2 modifiable: (the lists of cells or faces defining these "parts" can be changed over time)
- `NTCHRL`: default output frequency associated with this "writer" (the output may be forced or prevented at every time step using the subroutine `usnpst`)

In order to allow the user to add a supplementary output format to the main output format, or to add a supplementary mesh to the default output, the lists of standard and user meshes and "writers" are not separated. Negative numbers are reserved for the non-user items. For instance,the mesh numbers -1 and -2 correspond respectively to the global mesh and to boundary faces, generated by default, and the "writer" -1 corresponds to the usual post-processing case defined *via* `usini1` or *via* the interface.

The user chooses the numbers corresponding to the post-processing meshes and "writers" he wants to create. These numbers must be positive integers. It is possible to assocate a user mesh with the standard post-processing case (-1), or to ask for outputs concerning the boundary faces (-2) associated with a user "writer".

For safety, the output frequency and the possibility to modify the post-processing meshes are associated with the "writers" rather than with with the "parts". This logic avoids unwanted generation of inconstitent post-processing outputs. For instance EnSight would not be able to read a case in which one field is output to a given part every 10 time steps while another field is output to the same part every 200 time steps.

The possibility to modify a mesh over time is limited by the more restrictive "writer" which is associated with it. For instance, if the "writer" 1 allows the modification of the mesh topology (argument `INDMOD = 2` in the call to `PSTCWR`) and the "writer" 2 allows no modification (`INDMOD = 0`), a user post-processing mesh associated with the "writers" 1 and 2 will not be modifiable, but a mesh associated only with the "writer" 1 will be modifiable. The modification is done by means of the user subroutine `usmpst`, which is called only for the currently modifiable meshes.

It is also possible to define an alias of a post-processing mesh. An alias shares all the attributes of a "part" (without duplication), except its number. This may be used to output different variables on a same "part" with 2 different writers: the choice of output variables is based on the "part", so if P_a is associated with writer W_a, all that is needed is to define an alias P_b to P_a and associate it with writer W_b to allow a different output variable selection with each writer. An alias may be created using the `pstalm` subroutine.

Modification of a part or it's alias over time is always limited by the most restrictive "writer" to which it's meshes have been asscoiated (parts of the structures being shared in memory). It is possible to define as many alias' as are required for a "part", but an alias cannot be defined for another alias.

It is not possible to mix cells and faces in the same "part" (most of the post-processing tools being perturbed by such a case)[28]. If the user defines lists of faces and cells simultaneously, only the higher dimension entities (the cells) will be taken into account.

For a better understanding, the user may refer to the example given in `usdpst`. We can note that the whitespaces in the beginning or in the end of the character strings given as arguments of the functions called are suppressed automatically.

The variables to post-process on the defined "parts" will be specified in the subroutine `usvpst`. "

WARNING In the parallel case, some "parts" may not contain any local elements on a given processor. This is not a problem at all, as long as the "part" is defined for all processors (empty or not). It would in fact not be a good idea at all to define a "part" only if it contains local elements, global operations on the "part" would become impossible, leading to probable deadlocks or crashes.

4.27 Modification of the mesh zones to post-process: `usmpst`

Subroutine called only for each modifiable "part", at every active time step of an associated "writer".

For the user "parts" defined *via* the user subroutine `usdpst` and associated only with "writers" allowing the "part" modification over time (*i.e.* created with the parameter `INDMOD` = 2), this subroutine is

[28] in thr future, it will probably be possible to automatically add faces bearing group or attribute characteristics to a cell mesh, but those faces will only be written for formats supporting this (such as MED 2.2), and will only bear attributes, not variable fields

used to modify the lists of cells, internal and boundary faces defining this "part" (or post-processing mesh).

At first, the corresponding lists contain the previously defined values. If these lists are modified for a given post-processing mesh, the argument `IMODIF` must be given the value 1.If this argument maintains it's initial value of 0, the code will not consider this "part" to have been modified away from that call and it will offer to bring it upto date. It is in fact at the end of an optimisation so there is no need to modify these "parts" within the definate and modifiable assembly (if in doubt, let IMODIF=1).

It can be noticed that the indicator `ITYPPS` can be used to know whether the current post-processing mesh contains cells (`ITYPPS(1)` = 1), internal faces (`ITYPPS(2)` = 1), or boundary faces (`ITYPPS(2)` = 1)globally (as the number of local cells or faces of a processor could be 0, adn that doesn't provide sufficient information) . If at any instant in time, a given part contains no element of any type, all the values of ITYPES will be 0 and that number cannot be put in the part (`NUMMAI`) to dertimine if it will affect the cells or faces[29].

The user may refer to the example, in which cells are selected according to a given criterion:
- For a volumetric "part", cells for which the velocity exceeds a certain value.
- For a surface "part", internal faces which are between a cell in which the velocity exceeds a certain value and a cell in which the velocity is lower than this value (and boundary faces neighboring a cell in which the velocity exceeds this value). This surface post-processing mesh corresponds therefore to an approximation of a velocity isosurface.

4.28 Definition of the variables to post-process: `usvpst`

Subroutine called for each "part", at every active time step of an associated "writer" (see ***`usdpst`****).*

For the parts defined in `usdpst`, the subroutine `usvpst` is used to specify the variables to post-process.

The output of a given variable is generated by means of a call to `psteva`, whose arguments are:

- `NUMMAI`: current "part" number (input argument in `usvpst`).
- `NAMEVR`: name to give to the variable.
- `IDIMT`: dimension of the variable (3 for a vector, 1 for a scalar).
- `IENTLA`: indicates if the stored arrays are "intertwined" or not:
  - → 0: not intertwined, in the form $\{x_1, x_2, ..., x_n, y_1, y_2, ..., y_n, z_1, z_2, ..., z_n\}$ (case of all variables defined in `RTP`).
  - → 1: intertwined, in the form $\{x_1, y_1, z_1, x_2, y_2, z_2, ..., x_n, y_n, z_n\}$ (case of the geometric parameters, like `XYZCEN`, `SURFBO`, ...).

  For a scalar variable, this argument does not matter.
- `IVARPR`: indicates if the variable is defined on the "parent" mesh or locally:
  - → 0: variable generated by the user in the given work arrays `TRACEL`, `TRAFAC`, and `TRAFBR` (whose size is respectively the number of cells, internal faces and boundary faces of the "part", ×3). The arrays `LSTCEL`, `LSTFAC`, and `LSTFBR` can be used to get the numbers corresponding to the cells, internal faces and boundary faces associated with the "part" and to generate the appropriate post-processing variable.
  - → 1: variable already defined in the main mesh ("parent" mesh of the "parts"), for example the variables in the RTP array. Instructions in the report which list`LSTCEL`, `LSTFAC`, and `LSTFBR`will be treated directly by the sub routine, avoiding unused copies and simplifying hte code

[29] It is not expressly forbidden to associate with the "part" the cells with a certain timestep and the faces with another, but this modification has not been tested

- `NTCABS`: absolute current time step number. If a negative value is given (usually -1), the variable will be regarded as time-independent (and we will have to make sure this call is only made once).
- `TTCABS`: current physical time value. It is not taken into account if `NTCABS` < 0.
- `TRACEL`: array containing the values of the variable at the cells. If `IVARPR` $= 1$, this argument will be replaced by the position of the beginning of the array on which the variable in defined, for instance `RTP(1, IU(1))` for the velocity of the phase 1.
- `TRAFAC`: equivalent of `TRACEL` for the internal faces.
- `TRAFBR`: equivalent of `TRACEL` for the boundary faces.

The user may refer to the example, which presents the different ways of generating an output of a variable.

WARNING: Apart from the time-independent variables, it is not recommended not to generate the same variables at every call (corresponding to an active time step) for a given mesh, because the post-processing tool may have difficulties to deal with such a case. To generate outputs of different variables on the same mesh with different frequancies, it is recommended to create an alias of this mesh and to associate it with a different "writer" in the subroutine ***`usdpst`****.*

4.29 Modification of the variables at the end of a time step: `usproj`

Subroutine called every time step.

This subroutine is called at the end of every time step. It is used to print of modify any variable at the end of every time step.

Several examples are given:

- Calculation of a thermal balance at the boundaries and in the domain (including the mass source terms)
- Modification of the temperature in a given area starting from a given time
- Extraction of a 1D profile
- Printing of a moment
- Utilisation of the tool subroutines useful in the case of a parallel calculation (calculation of a sum on the processors, of a maximum, ...)

WARNING: As all the variables (solved variables, physical properties, geometric parameters) can be modified in this subroutine, a wrong use may distort totally the calculation.

The thermal balance example is particularly interesting.

- It can be easily adapted to another scalar (only three simple modifications to do, as indicated in the subroutine).
- It shows how to make a sum on all the subdomains in the framework of a parallel calculation (see the calls to the subroutines `PAR*`).
- It shows the precautions to take before doing some operations in the framework of periodic or parallel calculations (in particular when we want to calculate the gradient of a variable or to have access to values at the cells neighboring a face).
- Finally it must not be forgotten that the solving with temperature as a solved variable is questionable when the specific heat is not constant.

4.30 Radiative thermal transfers in semi-transparent gray media

4.30.1 Initialisation of the radiation main key words: `usray1`

Subroutine called only during calculation initialisation.

This subroutine is one of the two which must be completed by the user for all calculations including radiative thermal transfers. This subroutine is composed of three headings. The first one is dedicated to the activation of the radiation module, only in the case of classic physics.
WARNING: when a calculation is run using a specific physics module, this first heading must not be completed. The radiation module is then activated or not according to the parameter file related to the considered specific physics.

In the second heading the basic parameters of the radiation module are indicated.
Finally, the third heading deals with the selection of the post-processing graphic outputs. The variables to treat are splitted into two categories: the volumetric variables and those related to the boundary faces.

For more details about the different parameters, the user may refer to the key word list (§5).

4.30.2 Management of the radiation boundary conditions: `usray2`

Subroutine called every time step.

This is the second subroutine is necessary for every calculation including radiative thermal transfers. It is used to give all the necessary parameters concerning, in the one case, the wall temperature calculation, and in the other, the coupling between the termal scalar (temperature or enthalpy) and the radiation module at the calculation domain boundaries. It must be noted that the boundary conditions concerning the thermal scalar which may have been defined in the subroutine `usclim` will be modified by the radiation module according to the data given in `usray2` (cf. §4.2).
A zone number must be given to each boundary face [30]and, specifically for the walls, a boundary condition type and an initialisation temperature (in Kelvin). The initialisation temperature is only used to make the solving implicit at the first time step. The zone number allows to assign an arbitrary integer to a set of boundary faces having the same radiation boundary condition type. This gathering is used by the calculation, and in the listing to print some physical values (mean temperature, net radiative flow ...). An independent graphic output in *EnSight* format is associated with each zone and allows the display on the boundary faces of the variables selected in the third heading of the subroutine `usray1`.
A boundary condition type stored in the array ISOTHP is associated with each boundary face. There are five different types:

- **ITPIMP**: wall face with imposed temperature,
- **IPGRNO**: for a gray or black wall face, calculation of the temperature by means of a flux balance,
- **IPREFL**: for a reflecting wall face, calculation of the temperature by means of a flux balance, . This is fixed at 2000 in `radiat.h` and cannot be modified.
- **IFGRNO**: gray or black wall face to which a conduction flux is imposed,
- **IFREFL**: reflecting wall face to which a conduction flux is imposed, which is equivalent to impose this flux directly to the fluid.

[30]this must be less than the maximum allowable by the code, `NOZRDM`. This is fixed at 2000 in `radiat.h` and cannot be modified.

Depending on the selected boundary condition type at every wall face, the code needs to be given some supplementary pieces of information:

- **ITPIMP**: the array TINTP must be completed with the imposed temperature value and the array EPSP must be completed with the emissivity value (strictly positive).
- **IPGRNO**: must be given: an initialisation temperature in the array TINTP, the wall emissivity (strictly positive, in EPSP), thickness (in EPAP), thermal conductivity (in XLAMP) and an external temperature (in TEXTP) in order to calculate a conduction flux across the wall.
- **IPREFL**: must be given: an initialisation temperature (in TINTP), the wall thickness (in EPAP) and thermal conductivity (in XLAMP) and an external temperature (in TEXTP).
- **IFGRNO**: must be given: an initialisation temperature (in TINTP), the wall emissivity (in EPSP) and the conduction flux (in W/m^2 whatever the thermal scalar, enthalpy or temperature) in the array RCODCL. The value of RCODCL is positive when the conduction flux is directed from the inside of the fluid domain to the outside (for instance, when the fluid heats the walls). If the conduction flux is null, the wall is adiabatic.
- **IFREFL**: must be given: an initialisation temperature (in TINTP) and the conduction flux (in W/m^2 whatever the thermal scalar) in the array RCODCL. The value of RCODCL is positive when the conduction flux is directed from the inside of the fluid domain to the outside (for instance, when the fluid heats the walls). If the conduction flux is null, the wall is adiabatic. The flux received by RCODCL is directly imposed as boundary condition for the fluid.

WARNING: it is obligatory to set a zone number to every boundary face, even those which are not wall faces. These zones will be used during the printing in the listing. It is recommended to gather together the boundary faces of the same type, in order to ease the reading of the listing.

4.30.3 Absorption coefficient of the medium, boundary conditions for the luminance and calcualtion of the net radiative flux: `usray3`

Subroutine called every time step.

This subroutine is composed of three parts. In the first one, the user must provide the absorption coefficient of the medium in the array CK, for each cell of the fluid mesh. By default, the absorption coefficient of the medium is 0, which corresponds to a transparent medium.

WARNING: when a specific physics is activated, it is forbidden to give a value to the absorption coefficient in this subroutine. In this case, it is calculated automatically, or given by the user via *a thermo-chemical parameter file (dp_C3P or dp_C3PSJ for gas combustion, and dp_FCP for pulverised coal combustion).*

The two following parts of this subroutine concern a more advanced use of the radiation module. It is about imposing boundary conditions to the equation of radiative transfer and net radiative flux calculation, in coherence with the luminance at the boundary faces, when the user wants to give it a particular value. In most cases, the given examples do not need to be modified.

4.30.4 Encapsulation of the temperature-enthalpy conversion: `usray4`

Subroutine called every time step.

This subroutine is used to call the subroutine `usthht`. The user can implement his own conversion formulas into it.

This subroutine is useless when the thermal scalar is the temperature.

WARNING: when a specific physics is activated, it is forbidden to use this subroutine. In this case, `usray4` *is replaced by* `ppray4`*, which is not a user subroutine.*

The value of the argument MODE allows to know in which direction the conversion will be made:

- **MODE = 1**: the fluid enthalpy in the cell must be converted into temperature (in Kelvin),
- **MODE = -1**: the wall temperature (TEXT or TPAROI, in Kelvin) must be converted into enthalpy.

WARNING: the value of MODE is passed as argument and must not be modified by the user.

4.31 Utilisation of a specific physics: `usppmo`

Subroutine called only during calculation initialisation.

This is one of the three subroutines which must be obligatory completed by the user in order to use a specific physics module. At the moment, *Code_Saturne* allows to use two "pulverised coal" modules (lagrangian coupling or not), two "gas combustion" modules, two "electric" modules and one "compressible" module. To activate one of these modules, the user needs to complete one (and only one) of the indicators IPPMOD(I.....) in the subroutine `usppmo`. By default, all the indicators IPPMOD(I.....) are initialised at -1, which means that no specific physics is activated.

- Diffusion flame in the framework of "3 points" rapid complete chemistry: indicator **IPPMOD(ICOD3P)**
  - → IPPMOD(ICOD3P) = 0 adiabatic conditions
  - → IPPMOD(ICOD3P) = 1 permeatic conditions (enthalpy transport)
  - → IPPMOD(ICOD3P) =-1 module not activated
- Eddy Break Up pre-mixed flame: indicator **IPPMOD(ICOEBU)**
  - → IPPMOD(ICOEBU) = 0 adiabatic conditions at constant richness
  - → IPPMOD(ICOEBU) = 1 permeatic conditions at constant richness
  - → IPPMOD(ICOEBU) = 2 adiabatic conditions at variable richness
  - → IPPMOD(ICOEBU) = 3 permeatic conditions at variable richness
  - → IPPMOD(ICOEBU) =-1 module not activated
- Libby-Williams pre-mixed flame: indicator **IPPMOD(ICOLWC)**
  - → IPPMOD(ICOLWC)=0 two peak model with adibiatic conditions.
  - → IPPMOD(ICOLWC)=1 two peak model with permeatic conditions.
  - → IPPMOD(ICOLWC)=2 three peak model with adibiatic conditions.
  - → IPPMOD(ICOLWC)=3 three peak model with permeatic conditions.
  - → IPPMOD(ICOLWC)=4 four peak model with adibiatic conditions.
  - → IPPMOD(ICOLWC)=5 four peak model with permeatic condintions.
  - → IPPMOD(ICOLWC)=-1 module not activated.
- Multi-coals and multi-classes pulverised coal combustion: indicator **IPPMOD(ICP3PL)** The number of different coals must be inferior or equal to NCHARM = 3. The number of particle size classes NCLPCH(ICHA) for the coal ICHA, must be inferior or equal to NCPCMX = 10.

→ IPPMOD(ICP3PL) = 0 imbalance between the temperature of the continuous and the solid phases

→ IPPMOD(ICP3PL) = 1 otherwise

→ IPPMOD(ICP3PL) =-1 module not activated

- Lagrangian modeling of multi-coals and multi-classes pulverised coal combustion: indicator **IPPMOD(ICPL3C)** The number of different coals must be inferior or equal to NCHARM = 3. The number of particle size classes NCLPCH(ICHA) for the coal ICHA, must be inferior or equal to NCPCMX = 10.

  → IPPMOD(ICPL3C) = 1 coupling with the lagrangian module, with transport of H_2

  → IPPMOD(ICPL3C) =-1 module not activated

- Electric arc module (Joule effect and Laplace forces): indicator **IPPMOD(IELARC)**

  → IPPMOD(IELARC) = 1 determination of the magnetic field by means of the Ampere's theorem (not available)

  → IPPMOD(IELARC) = 2 determination of the magnetic field by means of the vector potential

  → IPPMOD(IELARC) =-1 module not activated

- Joule effect module (Laplace forces not taken into account): indicator **IPPMOD(IELJOU)**

  → IPPMOD(IELJOU) = 1 use of a real potential

  → IPPMOD(IELJOU) = 2 use of a complex potential

  → IPPMOD(IELJOU) = 3 use of real potential and specific boundary conditions for transformers.

  → IPPMOD(IELJOU) = 4 use of complex potential and specific boundary conditions for transformers.

  → IPPMOD(IELJOU) =-1 module not activated

- Compressible module: indicator **IPPMOD(ICOMPF)**

  → IPPMOD(ICOMPF) = 0 module activated

  → IPPMOD(ICOMPF) =-1 module not activated

WARNING: Only one specific physics module can be activated at the same time.

In the framework of the gas combustion modeling, the user may impose his own enthalpy-temperature tabulation (conversion law). He needs then to give the value zero to the indicator INDJON (the default value being 1). For more details, the user may refer to the following note (thermo-chemical files).

NOTE: THE THERMO-CHEMICAL FILES

The user must not forget to place in the directory DATA the thermo-chemical file `dp_FCP`, `dp_C3P`, `dp_C3PSJ` or `dp_ELE` (depending on the specific physics module he activated) and to specify the name of this file in the variable DONNEES_THERMOCHIMIE in the launch script (for instance: DONNEES_THERMOCHIMIE="dp_C3P"). Some example files are placed in the directory `DATA/THCH` at the creation of the study case. Their content is described below.

- Example of file for the gas combustion:

  → if the enthalpy-temperature conversion data base JANAF is used: `dp_C3P` (see array1).

  → if the user provides his own enthalpy-temperature tabulation (there must be three chemical species and only one reaction): `dp_C3PSJ` (see array 2). This file replaces `dp_C3P`.

- Example of file for the pulverised coal combustion: `dp_FCP` (see array 3).

- Example of file for the electric arc: `dp_ELE` (see array 4).

Lines	Examples of values	Variables	Observations
1	5	NGAZE	Number of current species
2	10	NPO	Number of points for the enthalpy-temperature tabulation
3	300.	TMIN	Temperature inferior limit for the tabulation
4	3000.	TMAX	Temperature superior limit for the tabulation
5			Empty line
6	CH4 O2 CO2 H2O N2	NOMCOE(NGAZE)	List of the current species
7	0	IRAYPP	0: no radiation 1: calculation of the absorption coefficient CKABS from the absorption coefficient KABSE of the current species 2: calculation using Modak 3: like 1 but P-1 model 4: like 2 but P-1 model
8	.35 .35 .35 .35 .35	KABSE(NGAZE)	Absorption coefficient of the current species
9	4	NATO	Number of elemental species
10 11 12 13	.012 1 0 1 0 0 .001 4 0 0 2 0 .016 0 2 2 1 0 .014 0 0 0 0 2	WMOLAT(NATO), ATGAZE(NGAZE,NATO)	Molar mass of the elemental species (first column) Composition of the current species as a function of the elemental species (NGAZE following columns)
14	3	NGAZG	Number of global species Here, NGAZG = 3 (Fuel, Oxidiser and Products)
15 16 17	1. 0. 0. 0. 0. 0. 1. 0. 0. 3.76 0. 0. 1. 2. 7.52	COMPOG(NGAZE,NGAZG)	Composition of the global species as a fonction of the current species of the line 6 In the order: Fuel (line 15), Oxidiser (line 16) and Product (line 17)
18	1	NRGAZ	Number of global reactions Here NRGAZ = 1 (always equal to 1 in this version)
19	1 2 -1 -9.52 10.52	IGFUEL(NRGAZ), IGOXY(NRGAZ), STOEG(NGAZG,NRGAZ)	Numbers of the global species concerned by the stoichiometric ratio (first 2 integers) Stoichiometry in reaction global species. Negative for the reactants (here "Fuel" and "Oxidiser") et positive for the products (here "Products")

Table 1: Example of file for the gas combustion when JANAF is used: `dp_C3P`

Lines	Examples of values	Variables	Observations
1	6	NPO	Number of tabulation points
2 3 4 5 6 7	50. -0.32E+07 -0.22E+06 -0.13E+08 250. -0.68E+06 -0.44E+05 -0.13E+08 450. 0.21E+07 0.14E+06 -0.13E+08 650. 0.50E+07 0.33E+06 -0.12E+08 850. 0.80E+07 0.54E+06 -0.12E+08 1050. 0.11E+08 0.76E+06 -0.11E+08	TH(NPO), EHGAZG(1,NPO), EHGAZG(2,NPO), EHGAZG(3,NPO)	Temperature(first column), mass enthalpy of fuel, oxidiser and products (columns 2,3 and 4) from line 2 to line NPO+1
8	.00219 .1387 .159	WMOLG(1), WMOLG(2), WMOLG(3)	Molar mass of fuel, oxidiser and products
9	.11111	FS(1)	Mixing rate at the stoichiometry (relating to Fuel and Oxidiser)
10	0	IRAYPP	0: no radiation 1: calculation of the absorption coefficient CKABS from the absorption coefficient KABSG of the 3 global species (Fuel, Oxydise, Products) 2: calcul using Modak 3: like 1 but P-1 model 4: like 2 but P-1 model
11	0.4 0.5 0.87	CKABSG(1), CKABSG(2), CKABSG(3)	Absorption coefficient of fuel, oxidiser and products
12	1. 2.	XCO2, XH2O	Molar coefficents of CO_2 and H_2O in the products (radiation using Modak)

Table 2: Example of file for the gas combustion when the user provides his own enthalpy-temperature tabulation (there must be three species and only one reaction): `dp_C3PSJ` (this file replaces `dp_C3P`)

Lines	Examples of values	Variables	Observations
1	THERMOCHIMIE		Comment line
2	8	NCOEL	Number of current species
3	8	NPO	Number of points for the enthalpy-temperature tabulation
4	ESPECES COURANTES		Comment line
5	CH4 C2H4 CO O2 CO2 H2O N2 C(S)	NOMCOEL(NCOEL)	List of the current species
6	300.	TMIN	Temperature inferior limit (Kelvin) for the enthalpy-temperature tabulation
7	2400.	TMAX	Temperature superior limit (Kelvin) for the enthalpy-temperature tabulation
8	4	NATO	Number of elemental species
9 10 11 12	.012 1 2 1 0 1 0 0 1 .001 4 4 0 0 0 2 0 0 .016 0 0 1 2 2 1 0 0 .014 0 0 0 0 0 0 0 2 0	WMOLAT(NATO), ATCOEL(NCOEL,NATO)	Molar mass of the elemental species (first column) and composition of the current species as a function of the elemental species
13	RAYONNEMENT		Comment line
14	1	IRAYPP	0: no radiation 1: constant, given below 2: using Modak 3: like 1 but P-1 model 4: like 2 but P-1 model
15	0.1	CKABS1	Constant absorption coefficient for the gas mixture
16	CARACTERISTIQUES CHARBONS		Comment line
17	2	NCHARB	Number of coal types
18	1 1	NCLPCH(NCHARB)	Number of classes for each coal (each column corresponding to one coal type)
19	50.E-6 50.E-6	DIAM20(NCLACP)	Initial diameter of each class (m) NCLACP is the total number of classes. All the diameters are written on the same line (sucessively for each coal, we give the diameter corresponding to each class)
20	74.8 60.5	CCH(NCHARB)	Composition in C (mass.-%, dry) of each coal
21	5.1 4.14	HCH(NCHARB)	Composition in H (mass.-%, dry) of each coal
22	12.01 5.55	OCH(NCHARB)	Composition in O (mass.-%, dry) of each coal
23	0 31524000. 0 31524000.	IPCI(NCHARB), PCICH(NCHARB)	Value of the PCI (Jkg^{-1}) for each coal, the first integer indicating if this value refers to pure (0) or dry coal (1)
24	1800. 1800.	CP2CH(NCHARB)	Heat-storage capacity at constant pressure ($Jkg^{-1}K^{-1}$) for each coal
25	1200. 1200.	RHO0CH(NCHARB)	Initial density (kgm^{-3}) of each
26	Coke		Comment line
27	0. 0.	CCK(NCHARB)	Composition in C (mass.-%, dry) of the coke for each coal
28	0. 0.	HCK(NCHARB)	Composition in H (mass.-%, dry) of the coke for each coal
29	0. 0.	OCK(NCHARB)	Composition in O (mass.%, dry) of the coke for each coal
30	0. 0.	PCICK(NCHARB)	PCI of the dry coke (Jkg^{-1}) for each coal
31	Cendres		Comment line
32	6.3 6.3	XASHCH(NCHARB)	Ash mass fraction (mass.-%, dry) in each coal
33	0. 0.	H0ASHC(NCHARB)	Ash formation enthalpy (Jkg^{-1}) for each coal
34	0. 0.	CPASHC(NCHARB)	CP of the ashes ($Jkg^{-1}K^{-1}$) for each coal
35	Dévolatilisation (Kobayashi)		Comment line
36	1 0.37 0 0.37	IY1CH(NCHARB), Y1CH(NCHARB)	For each coal, pairs (IY1CH, Y1CH). The real Y1CH is the adimensional stoich. coefficient If the integer IY1CH is worth 1, the provided value of Y1CH is adopted and the composition of the light volatile matters is calculated automatically. If the integer IY1CH is worth 0, the provided value of Y1CH is ignored: Y1CH is calculated automatically (the light volatiles are then composed of CH_4, CO).
37	1 0.74 1 0.74	IY2CH(NCHARB), Y2CH(NCHARB)	For each coal, pairs (IY2CH, Y2CH). The real Y2CH is the adimensional stoich. coefficient If the integer IY2CH is worth 1, the provided value of Y2CH is adopted and the composition of the heavy volatile matters is calculated automatically. If the integer IY2CH is worth 0, the provided value of Y2CH is ignored: Y2CH is calculated automatically (the heavy volatiles are then composed of C_2H_4, CO).
38	370000. 410000.	A1CH(NCHARB)	Devolatilisation pre-exponential factor A1 (s^{-1}) for each coal (light volatile matters)
39	1.3E13 1.52E13	A2CH(NCHARB)	Devolatilisation pre-exponential factor A2 (s^{-1}) for each coal (heavy volatile matters)
40	74000. 80000.	E1CH(NCHARB)	Devolatilisation activation energy E1 ($Jmol^{-1}$) for each coal (light volatile matters)
41	250000. 310000.	E2CH(NCHARB)	Energie d'activation E2 ($Jmol^{-1}$) de dévolatilisation for each coal (heavy volatile matters)
42	Combustion hétérogène		Ligne de commentaire
43	17.88 17.88	AHETCH(NCHARB)	Char burnout pre-exponential constant ($kgm^{-2}s^{-1}atm^{-1}$) for each coal
44	16.55 16.55	EHETCH(NCHARB)	Char burnout activation energy ($kcalmol-1$) for each coal
45	1 1	IOCHET(NCHARB)	Char burnout reaction order for each coal 0.5 if IOCHET = 0 and 1 if IOCHET = 1

Table 3: Example of file for the pulverised coal combustion: `dp_FCP`

Li nes	Examples of values	Variables	Observations
1	# Fichier ASCII format libre ...		Free comment
2	# Les lignes de commentaires ...		Free comment
3	# ...		Free comment
4	# Proprietes de l'Argon ...		Free comment
5	# ...		Free comment
6	# Nb d'especes NGAZG et Nb ...		Free comment
7	# NGAZG NPO ...		Free comment
8	1 238	NGAZG NPO	Number of species Number of given temperature points for the tabulated physical properties (NPO $\leqslant$ NPOT set in ppthch.h) So there will be NGAZG blocks of NPO lines each
9	# ...		Free comment
10	# Proprietes ...		Free comment
11	# T H ...		Free comment
12	# Temperature Enthalpie ...		Free comment
13	# ...		Free comment
14	# K J/kg ...		Free comment
15	# ...		Free comment
16	300. 14000. ...	 H ROEL CPEL SIGEL VISEL XLABEL XKABEL	Tabulation in line of the physical properties as a function of the temperature in Kelvin for each of the NGAZG species Enthalpy in J/kg Density in kg/m3 Specific heat in J/(kg K) Electric conductivity in Ohm/m Dynamic viscosity in kg/(m s) Thermal conductivity in W/(m K) Absorption coefficient (radiation)

Table 4: Example of file for the electric arc module: `dp_ELE`

4.32 Management of the boundary conditions related to pulverised coal and gas combustion: `usebuc, usd3pc, uslwcc, uscpcl et uscplc`

Subroutines called every time step.

In this paragraph, "specific physics" refers to gas combustion or to pulverised coal combustion.

As are `usini1` and `usppmo`, the use of `usebuc`, `usd3pc`, `uslwcc`, `uscpcl` or `uscplc` is obligatory to run a calculation concerning a specific physics modeling. The way of using them is the same as the way of using `usclim` in the framework of standard calculations, that is to say several loops on the boundary faces lists (cf. §4.2) marked out by their colors, groups, or geometrical criterion, where the type of face, the type of boundary condition for each variable and eventually the value of each variable are defined.

WARNING: In the case of a specific physics modeling, all the boundary conditions for every variable must be defined here, even for the eventual user scalars: `usclim` *is not used at all.*

In the case of a specific physics modeling, a zone number IZONE [31] (for instance the color ICOUL) is associated with every boundary face, in order to gather together all the boundary faces of the same type. In comparison to `usclim`, the main change from the user point of view concerns the faces whose boundary conditions belong to the type ITYPFB=IENTRE:

- for the EBU pre-mixed flame module:
  - → the user can choose between the "burned gas inlet" type (marked out by the burned gas indicator IENTGB(IZONE)=1) and the "fresh gas inlet" type (marked out by the fresh gas indicator IENTGF(IZONE)=1)
  - → for each inlet type (fresh or burned gas), a mass flow or a velocity must be imposed:
    - to impose the mass flow,
      - the user gives to the indicator IQIMP(IZONE) the value 1,
      - the mass flow value is set in QIMP(IZONE) (positive value, in kgs^{-1})
      - finally he imposes the velocity vector direction by giving the components of a direction vector in RCODCL(IFAC,IU(IPHAS)), RCODCL(IFAC,IV(IPHAS)) and RCODCL(IFAC,IW(IPHAS))

      WARNING:
      - *the variable QIMP(IZONE) refers to the mass flow across the whole zone IZONE and not across a boundary face (specifically for the axisymetric calculations, the inlet suface of the mesh must be broken up)*
      - *the variable QIMP(izone) deals with the inflow across the area IZOZ and only across this zone;it is recomended to pay attention to the boundary conditions.*
      - *the velocity direction vector is neither necessarily normed, nor necessarily incoming.*
    - to impose a velocity, the user must give to the indicator IQIMP(IZONE) the value 0 and set the three velocity components (in $m.s^{-1}$) in RCODCL(IFAC,IU(IPHAS)), RCODCL(IFAC,IV(IPHAS)) and RCODCL(IFAC,IW(IPHAS))
  - → finally he specifies for each gas inlet type the mixing rate FMENT(IZONE) and the temperature TKENT(IZONE) in Kelvin
- for the "3 points" diffusion flame module:
  - → the user can choose between the "oxydiser inlet" type marked out by IENTOX(IZONE)=1 and the "fuel inlet" type marked out by IENTFU(IZONE)=1

[31] IZONE must be less than the maximum number of boundary zone allowable by the code, NOZPPM. This is fixed at 2000 in `pppvar.h`;not to be modified

→ concerning the input mass flow or the input velocity, the method is the same as for the EBU pre-mixed flame module

→ finally, the user sets the temperatures TINOXY for each oxydiser inlet and TINFUE, for each fuel inlet

Note: In the standard version, only the cases with only one oxydising inlet type and one fuel inlet type can be treated. In particular, there must be only one input temperature for the oxidiser (TINOXY) and one input temperature for the fuel (TINFUEL).

- for the pulverised coal module:

→ the inlet faces can belong to the "primary air and pulverised coal inlet" type, marked out by IENTCP(IZONE)=1, or to the "secondary or tertiary air inlet" type, marked out by IENTAT(IZONE)=1

→ in a way which is similar to the process described in the framework of the EBU module, the user chooses for every inlet face to impose the mass flow or not (IQIMP(IZONE)=1 or 0). If the mass flow is imposed, the user must set the air mass flow value QIMPAT(IZONE), its direction in RCODCL(IFAC,IU(IPHAS)), RCODCL(IFAC,IV(IPHAS)) and RCODCL(IFAC,IW(IPHAS)) and the incoming air temperature TIMPAT(IZONE) in Kelvin. If the velocity is imposed, he has to set RCODCL(IFAC,IU(IPHAS)), RCODCL(IFAC,IV(IPHAS)) and RCODCL(IFAC,IW(IPHAS)).

→ if the inlet belongs to the "primary air and pluverised coal" type (IENTCP(IZONE) = 1) the user must also define for each coal type ICHA: the mass flow QIMPCP(IZONE,ICHA), the granulometric distribution DISTCH(IZONE,ICHA,ICLAPC) related to each class ICLACP, and the injection temperature TIMPCP(IZONE,ICHA)

4.33 Initialisation of the variables related to pulverised coal and gas combustion: `usebui, usd3pi, uslwci and uscpiv`

Subroutines called only during the calculation initialisation.

In this paragraph, "specific physics" refers to gas combustion or to pulverised coal combustion.

These subroutines allow the user to initialise some variables specific to the specific physics activated *via* `usppmo`. As usual, the user may have access to several geometric variables to discriminate between different initialisation zones if needed.

WARNING: in the case of a specific physics modeling, all the variables will be initialised here, even the eventual user scalars: `usiniv` *is no longer used.*

- in the case of the EBU pre-mixed flame module, the user can initialise in every cell IEL: the mixing rate RTP(IEL,ISCA(IFM)) in variable richness, the fresh gas mass fraction RTP(IEL,ISCA(IYGFM)) and the mixture enthalpy RTP(IEL,ISCA(IHM)) in permeatic conditions

- in the case of the rapid complete chemistry diffusion flame module, the user can initialise in every cell IEL: the mixing rate RTP(IEL,ISCA(IFM)), its variance RTP(IEL,ISCA(IFP2M)) and the mixture mass enthalpy RTP(IEL,ISCA(IHM)) in permeatic conditions

- in the case of the pulverised coal combustion module, the user can initialise in every cell IEL:

→ the transport variables related to the solid phase

RTP(IEL,ISCA(IXCH(ICLA))) the reactive coal mass fraction related to the class ICLA (ICLA from 1 to NCLACP which is the total number of classes, *i.e.* for all the coal type)

RTP(IEL,ISCA(IXCK(ICLA))) the coke mass fraction related to the class ICLA

RTP(IEL,ISCA(INP(ICLA))) the number of particles related to class ICLA per kg of air-coal mixture

RTP(IEL,ISCA(IH2(ICLA))) the mass enthalpy related to the class ICLA in permeatic conditions

→ RTP(IEL,ISCA(IHM)) the mixture enthalpy

→ the transport variables related to the gas phase

RTP(IEL,ISCA(IF1M(ICHA))) the mean value of the tracer 1 representing the light volatile matters released by the coal ICHA

RTP(IEL,ISCA(IF2M(ICHA))) the mean value of the tracer 2 representing the heavy volatile matters released by the coal ICHA

RTP(IEL,ISCA(IF3M)) the mean value of the tracer 3 representing the carbon released as CO during coke burnout

RTP(IEL,ISCA(IF4P2M)) the variance associated with the tracer 4 representing the air (the mean value of this tracer is not transported, it can be deduced directly from the three others)

RTP(IEL,ISCA(IFP3M)) the variance associated with the tracer 3

4.34 Initialisation of the options of the variables related to pulverised coal and gas combustion: `usebu1, usd3p1, uslwc1, uscpi1 and uscpl1`

Subroutines called at calculation beginning.

In this paragraph, "specific physics" refers to gas combustion or pulverised coal combustion.

These 3 subroutines are used to complete `usini1` for the considered specific physics. They allow to:

- generate, for the variables which are specific to the activated specific physics module, chronological outputs (indicators ICHRVR(IPP)), follow-ups in the listings (indicator ILISVR(IPP)) and to activate chronological records at the probes defined in `usini1` (indicators IHISVR(IPP)). The way of doing it is the same as in `usini1` and the writing frequencies of these ouputs are set by `usini1`. The values of the indicators IPP are IPP=IPPPRO(IPPROC(IVAR)), with IVAR the number of the specific physics variable. Concerning the main variables (velocity, pressure, etc ...) the user must still complete `usini1` if he wants to get chronological records, printings in the listing or chronological outputs. The variables which can be activated by the user for each specific physics are listed below. The calculation variables IVAR (defined at the cell IEL by RTP(IEL,IVAR)) and the properties IPROP (defined at the cell IEL by PROPCE(IEL,IPPROC(IPROP))) are listed now:

  → EBU pre-mixed flame modeling:

  - Calculation variables RTP(IEL,IVAR)

    IVAR = ISCA(IYGFM) fresh gas mass fraction

    IVAR = ISCA(IFM) mixing rate

    IVAR = ISCA(IHM) enthalpy, if transported
  - Properties PROPCE(IEL,IPPROC(IPROP))

    IPROP = ITEMP temperature

    IPROP = IYM(1) fuel mass fraction

    IPROP = IYM(2) oxidiser mass fraction

    IPROP = IYM(3) product mass fraction

    IPROP = ICKABS absorption coefficient, when the radiation modeling is activated

    IPROP = IT3M and IT4M "T^3" and "T^4" terms, when the radiation modeling is activated

→ rapid complete chemistry diffusion flame modeling:

everything is identical to the "EBU" case, except from the fresh gas mass fraction which is replaced by the variance of the mixing rate IVAR=ISCA(IFP2M)

→ pulverised coal modeling with 3 comustables:

variables shared by the two phases:

- Calculation variables RTP(IEL,IVAR)
  IVAR = ISCA(IHM): gas-coal mixture enthalpy
  IVAR = ISCA(IMMEL): molar mass of the gas mixture

variables specific to the dispersed phase:

- Calculation variables RTP(IEL,IVAR)
  IVAR = ISCA(IXCK(ICLA)): coke mass fraction related to the class ICLA
  IVAR = ISCA(IXCH(ICLA)): reactive coal mass fraction related to the class ICLA
  IVAR = ISCA(INP(ICLA)): number of particles of the class ICLA per kg of air-coal mixture
  IVAR = ISCA(IH2(ICLA)): mass enthalpy of the coal of class ICLA, if we are in permeatic conditions
- Properties PROPCE(IEL,IPPROC(IPROP))
  IPROP = IMMEL: molar mass of the gas mixture
  IPROP = ITEMP2(ICLA): temperature of the particles of the class ICLA
  IPROP = IROM2(ICLA): density of the particles of the class ICLA
  IPROP = IDIAM2(ICLA): diameter of the particles of the class ICLA
  IPROP = IGMDCH(ICLA): disappearance rate of the reactive coal of the class ICLA
  IPROP = IGMDV1(ICLA): mass transfer caused by the release of light volatiles from the class ICLA
  IPROP = IGMDV2(ICLA): mass transfer caused by the release of heavy volatiles from the class ICLA
  IPROP = IGMHET(ICLA): coke disappearance rate during the coke burnout of the class ICLA
  IPROP = IX2(ICLA): solid mass fraction of the class ICLA

variables specific to the continuous phase:

- Calculation variables RTP(IEL,IVAR)
  IVAR = ISCA(IF1M(ICHA)): mean value of the tracer 1 representing the light volatiles released by the coal ICHA
  IVAR = ISCA(IF2M(ICHA)): mean value of the tracer 2 representing the heavy volatiles released by the coal ICHA
  IVAR = ISCA(IF3M): mean value of the tracer 3 representing the carbon released as CO during coke burnout
  IVAR = ISCA(IF4PM): variance of the tracer 4 representing the air
  IVAR = ISCA(IF3P2M): variance of the tracer 3
- Properties PROPCE(IEL,IPPROC(IPROP))
  IPROP = ITEMP1: temperature of the gas mixture
  IPROP = IYM1(1): mass fraction of CH_{X1m} (light volatiles) in the gas mixture
  IPROP = IYM1(2): mass fraction of CH_{X2m} (heavy volatiles) in the gas mixture
  IPROP = IYM1(3): mass fraction of CO in the gas mixture
  IPROP = IYM1(4): mass fraction of O_2 in the gas mixture
  IPROP = IYM1(5): mass fraction of CO_2 in the gas mixture
  IPROP = IYM1(6): mass fraction of H_2O in the gas mixture
  IPROP = IYM1(7): mass fraction of N_2 in the gas mixture

- set the relaxation coefficient of the density SRROM, with
  $\rho^{n+1} = SRROM * \rho^n + (1 - SRROM)\rho^{n+1}$
  (by default, the adopted value is SRROM = 0.8. At the beginning of a calculation, a sub-relaxation of 0.95 may reduce the numerical "schocks").
- set the dynamic viscosity DIFTL0. By default DIFTL0= 4.25 $kgm^{-1}s^{-1}$ (the dynamic diffusivity being the ratio between the thermal conductivity λ and the mixture specific heat C_p in the equation of enthalpy).
- set the value of the constant CEBU of the Eddy Break Up model (only in `usebu1`. By default CEBU=2.5)

4.35 Management of Boundary Conditions of the electric arc: `uselcl`

sub routine called at each time step.

As in the `usini1` and `usppmo`, the use of `usecl` is required to run an electric calculation. The main use is the same as occurs in `usclim` for the standard *Code_Saturne* calculations, for which different loops on the boundary faces is defined. Each faces list is built with the use of selection criteria (cf. §4.2), and is referenced by their group(s), their color(s) or geometrical criterions. The face type, the boundary conditions for each variable, and finally the value of each variable or imposed flow are fixed.

WARNING:for the electric module, , the boundary conditions of all the variables are defined here, even those of the eventual user scalars: `usclim` *is not used at all.*

For the electric module, each boundary face is associated with a number `IZONE` [32](the color ICOUL for example) in order to group together all the boundary faces of the same type. In the report `usclim`, the main change from the users point of view concerns the specification of the boundary conditions of the potential, which isn't implied by default. The Dirichlet and Neuman conditions must be imposed explicitly using ICODCL and RCODCL (as would be done for the classic scalar).

Whats more, if one wishes to slow down the power dissipation(Joule module effect) or the current (electric arc module) from the imposed values(PUISMP and COUIMP respectively), they can be changed by the potential scalar as shown below :

- For the electric arc, the imposed potential difference can be a fixed variable: for example, the cathode can be fixed at 0 and the potential at the anode contains the variable DPOT. This variable is initialised in `useli1` by an estimated potential difference. If IELCOR=1(see `useli1`), DPOT is updated automatically during the calcualtion to obtain the required current.
- For the Joule module effect, DPOT is again used with the same significane as it held in the electric arc module. If DPOT is not wanted in the setting of the boundary condtions, the variable COEJOU can be used. COEJOU is the coefficient by which the potential difference is multiplied to obtain the desired power dissipation . By default this begins at 1 and is updated automatically. If IELCOR-1 (see `useli1`), multiply the imposed potentials in `uselcl` by COEJOU at each time step to achieive the desired power dissipation.

WARNING: In alternative current, attention should be paid to the values of potential imposed at the limits: the variable named "real potential" represents an affective value if the current is in single phase, and a "real part" if not.

- For the Joule studies, a complex potential is someitmes needed (IPPMOD(IELJOU)=2): this is the case in particular where the current is in 3 phase. In affect, to have access to the phase of the potential, and not just its amplitude, the 2 variables must be deleted : in *Code_Saturne*, there are 2 arrays specified for this role, the real part and the imaginary part of the potential.

[32] `IZONE` must be less than the maximum value allowed by the code, NOZZPPM. This is fixed at 2000 in `ppvar.h` and cannot be modified.

For use in the code, these variables are named 'real potential' and 'imaginary potential'. For an alternative sinusoidal potential Pp, the maximum value is noted as $Pp_{\max}$, the phase is noted as ϕ, the real potential and the imaginary potential are respecively $Pp_{\max}\, cos\phi$ and $Pp_{\max}\, sin\phi$.

- For the Joule studies in which one does not have access to the phases, the real potential (imaginary part =0) will suffice (IPPMOD(IELJOU)=1): this is obviously the case with continous current, but also with single phase alternative current. In *Code_Saturne* there is only 1 varialbe for the potential, called "real potential". Pay attention to the fact that in alternate current, the "real potential" represents a effective value of potential , $\frac{1}{\sqrt{2}}\, Pp_{\max}$ (in continous current there is no such ambiguity).

4.36 Initialisation of the variables in the electric module

subroutine called only at the initialisation of the calculation

This subroutine allows the user to initialise some of the specific physics variables prompted via `usppmo` . The user has access, as usual, to many geometric variables so that the zones can be differentiated if needed.

WARNING: For the specific physics, it is here that all varialbes are initialsed: ***`usiniv`*** *is not used*

This subroutine works like `usiniv`. The values of potential and its constiuents are initialised if required.

It should be noted that the enthalpy is important.

- For the electric arc module, the enthalpy value is taken from the temperature of reference T0(IPHAS)(given is `usini1`) from the temperature-enthalpy tables supplied in the data file `dp_ELE`. The user must not intervene here.

- For the Joule effect module, the value of enthalpy must be specified by the user . An example is given of how to obtain the enthalpy from the temperature of reference T0 (IPHAS)(given in `usini1`), the the temperature-enthalpy low must be supplied. A code is suggested in the sub routine `usthht`(which is there for the determination of physical properties).

4.37 Initialisation of the variable options in the electric module

subroutine called at each time step

This subroutine is completed in `usini1` for the specific physics. It allows:

- Activates the variables in the specific physics module, the chronolgical outputs (indicators ICHRVR(IPP)), the listings (indicator (ILISVR(IPP)) and the historical exits at the probes defined in `usini1`(indicators IHISVR(IPP)). The functions are the same as in `usini1` and the script frequency of the exits are fixed using `usini1`. The indicators IPP are for the value IPP=IPPPRO (IPPROC(IVAR), with IVAR, the number of specific physics varibles. With the main variables which concern the user(velocity, pressure, etc), the user must always use `usini1` if the history,the listings or the chronological files are required. The variables which the user can activate are marked out. The number of variables in the calculation is given in IVAR (defined to the cells IEL and accessible by PROPCE IEL,IPPROC(IPROP)):

  → Electric Arc Module:

  - Calculation variables RTP(IEL,IVAR)
    IVAR = ISCA(IHM) enthalpy
    IVAR = ISCA(IPOTR) real potentiel
    IVAR = ISCA(IPOTVA(i))) solved components of the potential vector.

IVAR = ISCA(IYCOEL(IESP)) the mass fraction of NGAZG composites if there are more than 1

- Properties PROPCE(IEL,IPPROC(IPROP))

IPROP = ITEMP temperature

IPROP = IEFJOU power dissipation by the Joule effect.

IPROP = ILAPLA(i) components of the laplace forces.

→ Joule Module effect :

- Calculation variables RTP(IEL,IVAR)

IVAR = ISCA(IHM) enthalpy

IVAR = ISCA(IPOTR) real potential

IVAR = ISCA(IPOTI) imaginary potential if its to be taken into account

IVAR = ISCA(IYCOEL(IESP))the mass fraction of NGAZG composites if there are more than 1

- Properties PROPCE(IEL,IPPROC(IPROP))

IPROP = ITEMP temperature

IPROP = IEFJOU volumic power dissipation by Joule effect.

- to give the coefficient of relaxation of the density SRROM:
$\rho^{n+1} = SRROM * \rho^n + (1 - SRROM)\rho^n$
(for the electric arc, the sub-relaxation is taken into account during the 2nd time step; for the Joule effect the sub relaxation is not accounted for unless the user specifies in `uselph`

- indicates if the data will be fixed in the power dissipation or in the current, done in IELCOR.

- target current fixed as COUIMP(electric arc module) or the power dissipation PUISM (Joule module effect).

- Fix the initial value of potential difference DPOT, the for the calculations with a single fixed parameter as COUIMP or PUISM.

4.38 Management of variable physical properties in the electric module

Subroutine called at each time step

All the laws of the variation of physical data of the fluid are written (where neccessary) in this subroutine... The subroutine replaces `usphyyv` and a similar component.

WARNING: For the electric module, it is here that all the physical variables are defined (including the relative cells and the eventuel user scalars):`usepelph` is not used.

The user should ensure that the defined variation laws are valid for the whole range of variables. Particular attention should be taken with the non-linear laws (for example, a 3rd degree polynomial law giving negative values of density)

WARNING: with the electric module, all the physical propertie are assumed as variables and so are stored in the PROPCE array. CP0, VISCLS0,VISCL0 are not used

For the Joule effect, the user is obliged to supply the physical properties in the sub- routine. Examples are given which are to be adapted by the user. If the temperature is to be determined to calculate the physical properties, the solved variable, enthalpy must be deduced. The preffered temperature-enthalpy law can be selected in the subruotine `usthht` (an example of the interpolation is given from the law table. This subroutine can be re-used for the initialisation of the variables(`useliv`)) For the elecrtic arc module, the physical properties are intepolated from the data file `dp_ELE` supplied by the user. Modification is not generally necessary.

4.39 Management of the *EnSight* output in the electric module : `uselen`

Subroutine called at each chronological output

This subroutine allow the addition on N variables in the *EnSight* output file and works like the subroutine `usvpst` (with the electric module, it is however still possible to `usvpst`.

The algebraic variables related to the electric module are provided by default provided that they are not explicitely contained in the POPCE array:

- gradient of real potential in Vm^{-1} ($\underline{\text{grad}}\ Pot_R = -\underline{E}$)
- density of real current in Am^{-2} ($\underline{j} = \sigma \underline{E}$)

specifically for the Joule module effect with IPPMOD(IELJOU)=2 :

- gradient of imaginary potential in Vm^{-1}
- density of real current in Am^{-2}

specifically for the electric arc module with IPPMOD(IELARC)=2 :

- magnetic field in T ($\underline{\text{B}} = \underline{\text{rot}}\ \underline{\text{A}}$)

If it is convenient for the user, there is no need to add this subroutine into the FORT directory: the post-processing will be done automatically (at the same frequency (NTCHR) as the other calculation variables)

4.40 Compressible module

When the compressible module[33] is activated, it is recommended to:

- use the option "time step variable in time and uniform in space" (IDTVAR=1) with a maximum Courant number of 0.4 (COUMAX=0.4): these choices must be written in `usini1`
- keep the convective numerical schemes proposed by default.

4.40.1 Initialisation of the options of the variables related to the compressible module: `uscfx1` and `uscfx2`

Subroutine called every time step.

These subroutines complete `usini1`.

`uscfx1` allows to set non standard calculation options related to the compressible module, and in particular to fill in the key word ICFGRP allowing to take into account the hydrostatic equilibrium in the boundary conditions.

`uscfx2` allows to specify for the molecular thermal conductivity and the volumetric viscosity the following pieces of information:

- variable or not (IVISCV)
- reference value (VISCV0)

[33] For more details concerning the compressible version, the user may refer to the document "Implantation d'un algorithme compressible dans *Code_Saturne*", Rapport EDF 2003, HI-83/03/016/A, P. Mathon, F. Archambeau et J.-M. Hérard.

4.40.2 Management of the boundary conditions related to the compressible module: `uscfcl`

Subroutine called every time step.

The use of `uscfcl` is obligatory to run a calculation using the compressible module just as it is in both `usini1` and `usppmo` . The way of using it is the same as the way of using `usclim` in the framework of standard calculations, that is to say several loops on the boundary faces lists (cf. §4.2) marked out by their colors, groups, or geometrical criterion, where the type of face, the type of boundary condition for each variable and eventually the value of each variable are defined.

WARNING: in the case of a calculation using the compressible module, the boundary conditions of all the variables are defined here, even those of the eventual user scalars: `usclim` *is not used at all.*

In the compressible module, the different available boundary conditions are the followings:

- inlet/outlet for which everything is known
- supersonic outlet
- subsonic inlet
- subsonic wall
- wall
- symmetry

4.40.3 Ininitialisation of the variables related to the compressible module: `uscfxi`

Subroutine called only during calculation initialisation.

This subroutine is used to initialise some variables specific to the specific physics activated *via* `usppmo`. As usual, the user may have access to several geometric variables to discriminate between different initialisation zones if needed.

WARNING: in the case of a specific physics modeling, all the variables are initialised here: `usiniv` *is not used at all.*

This subroutine works like `usiniv` for velocity, turbulence and passive scalars. Concerning pressure, density, temperature and specific total energy, only 2 variables out of the 4 are independant. The user may also initialise the variable pair he wants (apart from temperature-energy) and the two other variables will be calculated automatically by giving the right value to the variable ICCFTH used for the call to `uscfth`.

4.40.4 Compressible module thermodynamics: `uscfth`

This subroutine is called several times every time step (boundary conditions, physical properties, solving of the energy equation, ...).

This subroutine is used to set the thermodynamics parameters. By default, the perfect gas laws are implemented. If the user needs to use other laws (perfect gas with variable Gamma, Van der Waals), he must modify this subroutine.

4.40.5 Management of the variable physical properties in the compressible module: `uscfpv`

Subroutine called every time step.

If necessary, all the variation laws of the fluid physical properties (viscosity, specific heat, ...) are described here. This subroutine replaces and is similar to `usphyv`.

The user should make sure that the defined variation laws are valid for the whole variation range of the variables.

4.41 Lagrangian modeling of multiphasic flows with dipersed inclusions

4.41.1 Initialisation of the main key words in the lagrangian modeling: `uslag1`

Subroutine called only during calculation initialisation.

This is one of the two subroutines which must be completed in the case of a calculation modeling a lagrangian multiphasic flow. This subroutine gathers in different headings all the key word which are necessary to configure the lagrangian module. The different headings refer to:

- the global configuration parameters
- the specific physical models describing the particle behaviour
- the backward coupling (influence of the dispersed phase on the continuous phase)
- the numerical parameters
- the volumetric statistics
- the boundary statistics
- the postprocessing in trajectory mode

For more details about the different parameters, the user may refer to the key word list (§5.7).

The results of the lagangian module consist in some information about the particle cloud. These pieces of information are displayed in the form of statistics. It is therefore necessary to activate the calculation of the statistics at a given instant during the simulation. To do so, there are different strategies which are strongly related to the flow nature, stationary or not.
Except from the cases where the injection conditions depend on the time, it is generally recommended to realise a first lagrangian calculation whose aim is to get a nearly constant particle number in the calculation domain. In a second step, a calculation restart is done to calculate the statistics.
When the monophasic flow is stationary and the inclusion presence rate is low enough to neglect their influence on the continuous phase behaviour, it is better to realise a lagrangian calculation on a fixed field. It is then possible to calculate stationary volumetric statistics and to give a statistical weight higher than 1 to the particles, in order to reduce the number to treat while keeping the right concentrations.
Otherwise, when the continuous phase flow is stationary, but the backward coupling must be taken into consideration, it is still possible to activate stationary statistics.
When the continuous phase flow is non-stationary, it is no longer possible to use stationary statistics. To have correct statistics at every moment in the whole calculation domain, it is imperative to have an established particle seeding and it is recommended (when it is possible) not to impose statistical weights different from the unity.
Finally, when the complete model is used for the turbulent dispersion modeling, the user must make sure that the volumetric statistics are directly used for the calculation of the locally undisturbed fluid flow field.

When the thermal evolution of the particles is activated, the associated particulate scalars are always the inclusion temperature and the locally undisturbed fluid flow temperature expressed in degrees

Celsius, whatever the thermal scalar associated with the continuous phase is (temperature or enthalpy). If the thermal scalar associated with the continuous phase is the temperature in Kelvin, the unit change is done automatically. If the thermal scalar associated with the continuous phase is the enthalpy, the enthalpy-temperature conversion subroutine `usthht` must be completed for MODE=1, and must express temperatures in degrees Celsius.
In all cases, the thermal backward coupling of the dispersed phase on the continuous phase is adapted to the thermal scalar transported by the fluid.

WARNING: Up to now, parallelism and periodicity are not compatible with the lagrangian module. This compatibility will be soon implemented. It is however possible, in the framework of a lagrangian calculation on a fixed field, to realise in a first step the calculation of the continuous phase using parallelism, and to conduct in a second step the lagrangian calculation by doing a restart on only one processor.

4.41.2 Management of the boundary conditions related to the particles: `uslag2` and `uslain`

In the framework of the multiphasic lagrangrian modeling, the management of the boundary conditions concerns the particle behaviour when there is an interaction between its trajectory and a boundary face. These boundary conditions may be imposed independently of those concerning the eulerian fluid phase (they are of course generally coherent). The boundary condition zones are actually redefined by the lagrangian module (cf. §4.2), and a type of particle behaviour is associated with each one.
The management of the lagrangian boundary conditions is done by means of several user subroutines: `uslag2` for the classic conditions and `uslain` to specify profiles if necessary. Otherwise, the subroutine `uslabo` allows to define the type of particle/wall interaction. It will be described in a specific paragraph.

SUBROUTINE `USLAG2`

Subroutine called every time step.

It is the second indispensable subroutine for every calculation using the lagrangian module. The main numerical variables and "pointers" are described below.

IFRLAG(NFABOR) [IA] : In the lagrangian module, the user defines NFRLAG boundary zones from the color of the boundary faces, or more generally from their properties (colors, groups ...), from the boundary conditions defined in `usclim`, or even from their coordinates. To do so, the array IFRLAG(NFABOR) giving for each face IFAC the number IFRLAG(IFAC) corresponding to the zone to which it belongs, is completed. The zone numbers (*i.e.* the values of IFRLAG(IFAC)) are chosen freely by the user, but must be strictly positive integers inferior or equal to NFLAGM (parameter stored in lagpar.h, whose default value is 100). A zone type is associated with every zone; it will be used to impose global boundary conditions. *WARNING: it is essential that every boundary face belongs to a zone.*.

IUSNCL(NFLAGM) [IA] : For all the NFRLAG boundary zones previously identified, the number of classes NBCLAS[34] of entering particles is given: IUSNCL(IZONE) = NBCLAS. By default, the number of particle classes is zero. The maximum number of classes is NCLAGM (parameter stored in lagpar.h, whose default value is 20)..

IUSCLB(NFLAGM) [IA] : For all the NFRLAG boundary zones previously identified, a particle boundary condition type is given. There are two categories of particle boundary condition types: those predefined in the subroutine `uslabo` (marked out by the key words IENTRL, ISORTL, IREBOL, IDEPO1, IDEPO2, IDEPO3, IENCRL) and the user boundary condition types (marked out by the key words JBORD1 to JBORD5), whose

[34] a class is a set of particles sharing the same physical properties and the same characteristics concerning the injection in the calculation domain

corresponding particle behaviour must be defined in the subroutine `uslabo`.

- if IUSCLB(IZONE) = IENTRL, IZONE is a particle injection zone. For each particle class associated with this zone, some pieces of information must be given (see below). If a particle trajectory crosses an injection zone, then we consider that this particle leaves the calculation domain.
- if IUSCLB(IZONE) = ISORTL, the particles interacting with the zone IZONE leave the calculation domain.
- if IUSCLB(IZONE) = IREBOL, the particles undergo an elastic rebound on the boundary zone IZONE.
- if IUSCLB(IZONE) = IDEPO1, the particles settle definitevely on the boundary zone IZONE. These particles can not be put in suspension again, and we consider that they leave the calculation domaine.
- if IUSCLB(IZONE) = IDEPO2, the particles settle definitevely on the boundary zone IZONE, but they are kept in the calculation domain. This distinction with the type IDEPO1 is useful only when post-processings in movement mode (IFENSI2 = 1) are realised: the particles do not disappear after touching the boundary zone. However, using IDEPO2 type zones necessitates more memory than using IDEPO1 type zones.
- if IUSCLB(IZONE) = IDEPO3, the particles settle on the boudary zone IZONE, but can be put in suspension again depending on the local description of the continuous phase flow.
- if IUSCLB(IZONE) = IENCRL, the particles which are coal particles (if IPHYLA = 2) can become fouled up on the zone IZONE. The slagging is a IDEPO1 type deposit of the coal particle if a certain criterion is respected. Otherwise, the coal particle rebounds (IREBOL type behaviour). This boundary condition type is available if IENCRA = 1. A limit temperature TPRENC, a critical viscosity VISREF and the coal composition in mineral matters must be given in the subroutine `uslag1`. The slagging criterion given by default may be modified in the subroutine `uslabo`.
- if IUSCLB(IZONE) = JBORD1 to JBORD5, then the particle interaction with the boundary zone IZONE is given by the user. The particle behaviour associated with each type JBORD* must be defined in the subroutine `uslabo`.

IUSLAG(NCLAGM, NFLAGM, NDLAIM) [IA] : Some pieces of information must be given for each particle class associated with an injection zone. The first part consists in integers contained in the array IUSLAG. There are at the most NDLAIM integers. These pieces of information must be provided for each class ICLAS and each particle injection zone IZONE. They are marked out by means of "pointers":

→ IUSLAG(ICLAS,IZONE,IJNBP): number of particles to inject in the calculation domain per class and per zone.

→ IUSLAG(ICLAS,IZONE,IJFRE): injection period (expressed in number of time steps). If the period is null, then there is injection only at the first absolute lagrangian time step (including the restart calculations).

→ IUSLAG(ICLAS,IZONE,IJUVW): type of velocity condition:

- if IUSLAG(ICLAS,IZONE,IJUVW) = 1, the particle velocity vector is imposed, and its components must be given in the array RUSLAG (see below).

- if IUSLAG(ICLAS,IZONE,IJUVW) = 0, the particle velocity is imposed perpendicular to the injection boundary face and with the norm RUSLAG(ICLAS,IZONE,IUNO).
- if IUSLAG(ICLAS,IZONE,IJUVW) = -1, the particle injection velocity is equal to the fluid velocity at the center of the cell neighboring the injection boundary face.

→ IUSLAG(ICLAS,IZONE,INUCHL): when the particles are coal particles (IPHYLA = 2), this part of the array contains the coal index-number, between 1 and NCHARB (defined by the user in the thermo-chemical file dp_FCP, with NCHARB$\leqslant$NCHARM = 3).

RUSLAG(NCLAGM, NFLAGM, NDLAGM) [RA] : Some pieces of information must be given for each particle class associated with an injection zone. The second and last part consists in real numbers contained in the array RUSLAG. There are at the most NDLAGM such real numbers. These pieces of information must be provided for each class ICLAS and each particle injection zone IZONE. They are marked out by means of "pointers":

→ RUSLAG(ICLAS,IZONE,IUNO): norm of the injection velocity,
useful if IUSLAG(ICLAS,IZONE,IJUVW) = 0.

→ RUSLAG(ICLAS,IZONE,IUPT), RUSLAG(ICLAS,IZONE,IVPT),
RUSLAG(ICLAS,IZONE,IWPT): components of the particle injection vector,
useful if IUSLAG(ICLAS,IZONE,IJUVW) = 1.

→ RUSLAG(ICLAS,IZONE,IDEBT): allows to impose a particle mass flow. According to the number of injected particles, the particle statistical weight TEPA(NPT,JRPOI) is recalculated in order to respect the required mass flow (the number of injected particles does not change). When the mass flow is null, it is not taken into account.

→ RUSLAG(ICLAS,IZONE,IPOIT): particle statistical weight per class and per zone.

→ RUSLAG(ICLAS,IZONE,IDPT): particle diameter. When the particles are coal particles (IPHYLA = 2), this diameter is provided by the thermo-chemical file dp_FCP *via* the array DIAM20(ICLG), where ICLG is the "pointer" on the total class number (*i.e.* for all the coal types). When the standard deviation of the particle diameter is different from zero, this diameter becomes a mean diameter.

→ RUSLAG(ICLAS,IZONE,IVDPT): standard deviation of the injection diameter. To impose this standard deviation allows to respect granulometric distribution: the diameter of each particle is calculated from the mean diameter, the standard deviation and a gaussian random number. In this case, it is strongly recommended to intervene in the subroutine `uslain` to restrict the diameter variation range, in order to avoid aberrant values. If this standard deviation is null, then the particle diameter is constant per class and per zone.

→ RUSLAG(ICLAS,IZONE,IROPT): particle density. When the particles are coal particles (IPHYLA = 2), this density is set in the thermo-chemical file dp_FCP *via* the array RHO0CH(ICHA), where ICHA is the coal number.

→ RUSLAG(ICLAS,IZONE,ITPT): particle injection temperature in °C. Useful if IPHYLA = 1 and if ITPVAR = 1.

→ RUSLAG(ICLAS,IZONE,ICPT): particle injection specific heat. Useful if IPHYLA = 1 and if ITPVAR = 1. When the particles are coal particles (IPHYLA = 2), the specific heat is set in the thermo-chemical file dp_FCP *via* the array CP2CH(ICHA).

→ RUSLAG(ICLAS,IZONE,IEPSI): particle emissivity. Useful if IPHYLA = 1 and if ITPVAR = 1, and if the radiation module is activated for the continuous phase (note: when IPHYLA = 2, the coal particle emissivity is given the value 1).

→ RUSLAG(ICLAS,IZONE,IHPT): particle injection temperature in °C when these particles are coal particles. The array RUSLAG(ICLAS,IZONE,ITPT) is then no longer active. Useful if IPHYLA = 2.

→ RUSLAG(ICLAS,IZONE,IMCHT): mass of reactive coal. Useful if IPHYLA = 2.

→ RUSLAG(ICLAS,IZONE,IMCKT): mass of coke. This mass is null if the coal did not begin to burn before its injection. Useful if IPHYLA = 2.

IUSVIS(NFLAGM) [IA] : In order to display the variables at the boundaries defined in the subroutine `uslag1`, this array allows to select the boundary zones on which a display is wanted. To do so, a number is associated with each zone IZONE. If this number is strictly positive, the corresponding zone is selected ; if it is null, the corresponding zone is eliminated. If several zones are associated with the same number, they will be displayed together in the same selection with *EnSight*. Each selection will be split in *EnSight* parts according to the geometric types of the present boundary faces ((*i.e.* 'tria3', 'quad4' et 'nsided')..

SUBROUTINE `USLAIN`

Subroutine called every time step.

It is not obligatory to intervene in this subroutine.

`uslain` is used to complete `uslag2` when the particles must be injected in the domain according to fine constraints (profile, position ...): the arrays ETTP, TEPA and ITEPA can be modified here for the new particles (these arrays were previously completed automatically by the code from the data provided by the user in `uslag2`).

In the case of a more advanced utilisation, it is possible to modify here all the arrays ETTP, TEPA and ITEPA. The particles already present in the calculation domain are marked out by an index varying between 1 and NBPART. The particles entering the calculation domain at the current iteration are marked out by an index varying between NBPART+1 and NBPNEW.

4.41.3 Treatment of the particle/boundary interaction: `uslabo`

Subroutine called at every particle/boundary interaction.

It is not obligatory to intervene in this subroutine, but it is required in four different cases.

Firstly, an intervention is required when JBORD* type boundary conditions are used: it is then necessary to code in this subroutine the corresponding particle/boundary interactions.

Secondly, it is possible to select the particle/boundary interaction types (IREBOL, IDEPO1, ...) for which the user wants to save the wall statistics activated in the subroutine `uslag1`.

Thirdly, if user boundary statistics are activated *via* the key word NUSBOR in the subroutine `uslag1`, it is then necessary to program them in the subroutine `uslabo`. When the boundary statistics are stationary, these new boundary statistics are added using the array PARBOR. When they are non-stationary (number of lagrangian iterations lower than NSTBOR, or ISTTIO = 0), the array PARBOR is reset at every iteration.

Fourthly, when the user wants to modify the formulation of the wall slagging by the coal particles, it is then necessary to program the new laws in the subroutine `uslabo`.

CONSTRUCTION RULES OF A NEW PARTICLE/BOUNDARY INTERACTION

1. The real numbers KX, KY, KZ provide the coordinates of the intersection point between the current particle trajectory and the interacting boundary face.
2. If the user wants to modify the particle position, it can be done directly *via* the arrays ETTP and ETTPA:
   - new departure point of the current trajectory segment:
     ETTPA(NPT,JXP), ETTPA(NPT,JYP), ETTPA(NPT,JZP)
   - new arrival point of the current trajectory segment:
     ETTP(NPT,JXP), ETTP(NPT,JYP), ETTP(NPT,JZP)
3. The particle and the fluid velocities may be modified according to the desired interaction *via* the arrays VITPAR and VITFLU, they **must not** be modified *via* ETTP and ETTPA in this subroutine.
4. For a given interaction, it is necessary to specify the key word ISUIVI:
   - ISUIVI = 0 if the particle does not need to be followed in the mesh after the interaction between its trajectory and the boundary face (by default, it is the case for IENTRL, ISORTL, IDEPO1, IDEPO2) ;
   - ISUIVI = 1 to continue to follow the particle in the mesh after its interaction (by default, it is the case for IREBOL and IDEPO3). The value of ISUIVI may be a function of the particle and boundary state (for instance, ISUIVI = 0 or 1 depending on the physical properties for the interaction type IENCRL).
5. The array zone ITEPA(NPT,JISOR), containing the index-number of the cell where the particle is, must be updated. Generally:
   - ITEPA(NPT,JISOR) = IFABOR(KFACE) when the particle stays in the calculation domain (KFACE is the number of the interacting boundary face).
   - ITEPA(NPT,JISOR) = 0 to eliminate definitively the particle from the calculation domain.

NOTE: ORDER OF THE NUMERICAL SCHEME AFTER A PARTICLE/BOUNDARY INTERACTION

When a particle interacts with a boundary face, the integration order of the associated stochastic equations is always a first-order, even if a second-order scheme is used elsewhere.

4.41.4 Option of particle cloning/fusion: `uslaru`

Subroutine called every lagrangian iteration.

An intervention in this subroutine is required if the particle cloning/fusion option is activated *via* the key word IROULE. The importance function CROULE must then be completed.
The aim of this technique is to reduce the number of particles to treat in the whole flow and to refine the description of the particle cloud only where the user wants to get volumetric statistics more accurate than in the rest of the calculation domain.
The values given to the importance function are strictly positive real numbers allowing to classify the zones according to their importance. The higher the value given to the importance function, the more important the zone.

For instance, when a particle moves from a zone of importance 1 to a zone of importance 2, it undergoes a cloning: the particle is replaced by two identical particles, whose statistical weight is the half of the initial particle. When a particle moves from a zone of importance 2 to a zone of importance 1, it undergoes a fusion: the particle survives to its passing through with a probability of 1/2. A random dawing is used to determine if the particle will survive or disappear.

In the same way, when a particle moves from a zone of importance 3 to a zone of importance 7, it undergoes a cloning. The particle is cloned in Int(7/3)=2 or Int(7/3)+1=3 particles with a probability of respectively 1-(7/3-Int(7/3))=2/3 and 7/3-Int(7/3)=1/3. If the particle moves from a zone of importance 7 to a zone of importance 3, it undergoes a fusion: it survives with a probability of 3/7.

WARNING: The importance function must be a strictly positive real number in every cell

4.41.5 Manipulation of particulate variables at the end of an iteration and user volumetric statistics: `uslast` and `uslaen`

`uslast`*: subroutine called at the end of every lagrangian iteration*

`uslaen`*: subroutine called at every chronological output and every listing printing*

The subroutine `uslast` is called at the end of every lagrangian iteration, it allows therefore the modification of variables related to the particles, or the extraction and preparation of data to display in the listing or the post-processing.

An intervention in both subroutines `uslast` and `uslaen` is required if supplementary user volumetric statistics are wanted.

User volumetric statistics:

The volumetric statistics are calculated by means of the array STATIS. Two situations may happen:

- the calculation of the statistics is not stationary: STATIS is reset at every lagrangian iteration ;
- the calculation of the statistics is stationary: the array STATIS is used to store cumulated values of variables, which will be averaged at the end of the calculation in the subroutine `uslaen`.

According to the user parameter settings, it may happen that during the same calculation, the statistics will be non-stationary in a first part and stationary in second part.

- User volumetric statistics: subroutine `USLAST`

  In this subroutine, the variable whose volumetric statistic is wanted is stored in the array STATIS. In the framework of stationary statistics, the average itself is calculated in the subroutine `uslaen`. This average is obtained through the division of the cumulated value by:
  - either the duration of the stationary statistics calculation stored in the variable TSTAT,
  - or the number of particles in statistical weight.

  This method of averaging is applied to every piece in the listing and to the post-processing outputs.

- User volumetric statistics: subroutine `USLAEN`

  In this subroutine is calculated the average corresponding to the cumulated value obtained in the subroutine `uslast`. This subroutine is also used for the standard volumetric statistics. Several examples are therefore described.

4.41.6 User stochastic differential equations: `uslaed`

Subroutine called every lagrangian sub-step.

An intervention in this subroutine is required if supplementary user variables are added to the particle state vector (arrays ETTP and ETTPA).

The integration of the stochastic differential equations associated with supplementary particulate variables is done in this subroutine.
When the integration scheme of the stochastic differential equations is a first-order (NORDRE = 1), this subroutine is called once every lagrangian iteration, if it is a second-order (NORDRE = 2), it is called twice.

The solved stochastic differential equations must be written in the form:

$$\frac{d\Phi_p}{dt} = -\frac{\Phi_p - \Pi}{\tau_\phi}$$

where Φ_p is the I*th* supplementary user variable (NVLS in total) available in ETTP(NBPMAX, JVLS(I)) and in ETTPA(NBPMAX,JVLS(I)), τ_ϕ is a quantity homogen to a characteristic time, and Π is a coefficient which may be expressed as a function of the other particulate variables contained in ETTP and ETTPA.
In order to do the integration of this equation, the following parameters must be provided:

- τ_ϕ, equation characteristic time, in the array AUXL1 for every particle,
- Π , equation coefficient, in the array AUXL2. If the integration scheme is a first-order, then Π is expressed as a function of the particulate variables at the previous iteration, stored in the array ETTPA. If the chosen scheme is a second-order, then Π is expressed at the first call of the subroutine (prediction step NOR = 1) as a function of the variables at the previous iteration (stored in ETTPA), then at the second call (correction step NOR = 2) as a function of the predicted variables stored in the array ETTP.

If necessary, the thermal characteristic time τ_c, whose calculation can be modified by the user in the subroutine `uslatc`, is stored for each particle in the part TEMPCT(NBPMAX,1) of the array TEMPCT.

4.41.7 Particle relaxation time: `uslatp`

Subroutine called every lagrangian sub-step.

An intervention in this subroutine is not obligatory.

In this subroutine, the particle relaxation time may be modified according to the chosen formulation of the drag coefficient.
The particle relaxation time, modified or not by the user, is available in the array TAUP.

4.41.8 Particle thermal characteristic time: `uslatc`

Subroutine called every lagrangian sub-step.

An intervention in this subroutine is not obligatory.

In this subroutine, the particle thermal characteristic time may be modified according to the chosen correlation for the calculation of the Nusselt number.
The thermal characteristic time, modified or not by the user, is available in the zone TEMPCT(NBPMAX,1) of the array TEMPCT.

5 Key word list

The key words are classified under headings. For each key word of the Kernel of *Code_Saturne*, the following data are given:

Variable name Type Allowed values [Default] O/C Level
Description
Potential dependences

- **Variable name**: Name of the variable containing the key word.
- **Type**: A (Array), I (Integer), R (Real number), C (Character string).
- **Allowed values**: list or range of allowed values.
- **Default**: value defined by the code before any user modification (every key word has one). In some cases, a non-allowed value is given (generally -999 or -1.D12), to force the user to specify a value. If he does not do it, the code may:
  - automatically use a recommended value (for instance, automatical choice of the variables for which chronological records will be generated).
  - stop, if the key word is essential (for instance, value of the time step).
- **O/C**: Optional/Compulsory
  - O: optional key word, whose default value may be enough.
  - C: key word which must imperatively be specified (for instance, the time step).
- **Level**: L1, L2 ou L3
  - L1 (level 1): the users will have to modify it in the framework of standard applications. The L1 key words are written in bold.
  - L2 (level 2): the users may have to modify it in the framework of advanced applications. The L2 key word are all optional.
  - L3 (level 3): the developers may have to modify it ; it keeps its default value in any other case. The L3 key word are all optional.
- **Description**: key word description, with its potential dependences.

The L1 key words can be modifed through the Graphical Use Interface or in the `usini1` subroutine. L2 and L3 key words can only be modified through the `usini1` subroutine, even if they do not appear in the version proposed as example it the `FORT/USERS/base` directory.
It is however recommended not to modify the key words which do not belong to the L1 level.

The alphabetical key word list is displayed in the index, in the end of this report.

NOTES
• The notation "D" refers to a double precision real. For instance, 1.8D-2 means 0.018.
• The notation "GRAND" (which can be used in the code) corresponds to 1.D12.

5.1 Inputs-outputs

NOTES

- Two different files can have neither the same unit number nor the same name.
- ASCII files (also called "formatted" files, in opposition to "binary" files) are bigger, longer to write and to read, but can be used on every architecture (in particular, it is an asset for calculation restart files). However, *Code_Saturne* can automatically recognise and convert Big Endian/Little Endian files. It is therefore usually possible on a given architecture to use binary restart files generated on another architecture.

5.1.1 "Calculation" files

General

IMPGEO	I	strictly positive integer	[10]	O	L3
unit of the geometric file (if the Preprocessor is not used) useful if and only if IFOENV = 0					
FICGEO	C	string of 6 characters	[`geomet`]	O	L3
name of the geometric file (if the Preprocessor is not used) useful if and only if IFOENV = 0					
IMPAMO	I	strictly positive integer	[11]	O	L3
unit of the upstream restart file useful if and only if ISUITE = 1					
FICAMO	C	string of 13 characters	[`suiamo`]	O	L3
name of the main upstream restart file. Its "format" (ASCII or binary) is automatically determined by the code. useful if and only if ISUITE = 1					
FICAMX	C	string of 13 characters	[`suiamx`]	O	L3
name of the auxiliary upstream restart file. Its "format" (ASCII or binary) is automatically determined by the code. useful if and only if ISUITE = 1					
IMPSTP	I	strictly positive integer	[12]	O	L3
unit of the calculation interactive stop file always useful (because of the interactive character)					
FICSTP	C	string of 6 characters	[`ficstp`]	O	L3
name of the calculation interactive stop file (see p.17) always useful (because of the interactive characteristic)					
IMPAVA	I	strictly positive integer	[20]	O	L3
unit of the main downstream restart file always useful					
IMPAVX	I	strictly positive integer	[IMPAVA]	O	L3
unit of the auxiliary downstream restart file always useful					

FICAVA C string of 13 characters [suiava] O L3
name of the main downstream restart file
always useful

FICAVX C string of 13 characters [suiavx] O L3
name of the auxiliary downstream restart file
always useful

IFOAVA I 1 or 0 [0] O L2
indicator (1: formatted, 0: binary main downstream restart file)
always useful

IFOAVX I 1 or 0 [0] O L2
indicator (1: formatted, 0: binary auxiliary downstream restart file)
always useful

1D wall thermal module

IMPMT1 I strictly positive integer [IMPAMO] O L3
unit of the upstream restart file for the 1D wall thermal module
useful if and only if ISUIT1 = 1 and NFPT1D>0

FICMT1 C string of 13 characters [t1damo] O L3
name of the upstream restart file for the 1D wall thermal module. Its "format" (ASCII or binary) is automatically determinedby the code.
useful if and only if ISUIT1 = 1 and NFPT1D>0

IMPVT1 I strictly positive integer [IMPAVA] O L3
unit of the downstream restart file for the 1D wall thermal module
useful if and only if NFPT1D>0

FICVT1 C string of 13 characters [t1dava] O L3
name of the upstream restart file for the 1D wall thermal module
useful if and only if NFPT1D>0

IFOVT1 I 1 or 0 [IFOAVA] O L2
indicator (1: formatted, 0: binary downstream restart file for the 1D wall thermal module)
useful if and only if NFPT1D>0

Vortex method for LES

IMPMVO I strictly positive integer [IMPAMO] O L3
unit of the upstream restart file for the vortex method
useful if and only if ISUIVO = 1 et IVRTEX=1

FICMVO C string of 13 characters [voramo] O L3
name of the upstream restart file for the vortex method

Its "format" is always ASCII (this file has a different structure from the other restart files)
useful if and only if ISUIVO = 1 et IVRTEX=1

IMPVVO I strictly positive integer [IMPAVA] O L3
unit of the downstream restart file for the vortex method
useful if and only if IVRTEX=1

FICVT1 C string of 13 characters [vorava] O L3
name of the upstream restart file for the vortex method
Its "format" is always ASCII (this file has a different structure from the other restart files)
useful if and only if IVRTEX=1

IMPDVO I strictly positive integer [IMPAVA] O L3
unit of the FICVOR data files for the vortex method. These files have an ASCII format. Their number and names are specified by the user in the `usvort` subroutine. (Although it corresponds to an "upstream" data file, IMPDVO is initialised to IMPAVA because, in case of multiple vortex entries, it is opened at the same time as the FICMVO upstream restart file, which already uses the IMPAMO unit)
useful if and only if IVRTEX=1

RADIATION

IMPAMR I strictly positive integer [IMPAMO] O L3
unit of the radiation upstream restart file
useful if and only if ISUIRD = 1

FICAMR C string of 13 characters [rayamo] O L3
name of the radiation upstream restart file. Its "format" (ASCII or binary) is automatically determined by the code.
useful if and only if ISUIRD = 1

IMPAVR I strictly positive integer [IMPAVA] O L3
unit of the radiation downstream restart file
always useful in case of radiation modeling

FICAVR C string of 13 characters [rayava] O L3
name of the radiation downstream restart file
always useful in case of radiation modeling

IFOAVR I 1 or 0 [IFOAVA] O L2
indicator (1: formatted, 0:binary radiation downstream restart file)
always useful in case of radiation modeling

THERMOCHEMISTRY

IMPFPP I strictly positive integer [25] O L3
unit of the thermochemical data file
useful in case of gas or pulverised coal combustion or electric arc

FICFPP C string of 6 characters [dp_tch] O L3
name of the thermochemical data file. The launch script is designed to copy the user specified thermochemical data file in the temporary execution directory under the name dp_tch, for *Code_Saturne* to open it properly. Should the value of FICFPP be changed, the launch script would have to be adapted.
useful in case of gas or pulverised coal combustion

IMPJNF I strictly positive integer [IMPFPP] O L3
unit of the JANAF data file
useful in case of gas or pulverised coal combustion

FICJNF C string of 5 characters [JANAF] O L3
name of the JANAF data file. The launch script is designed to copy the user specified JANAF data file in the temporary execution directory under the name JANAF, for *Code_Saturne* to open it properly. Should the value of FICJNF be changed, the launch script would have to be adapted.
useful in case of gas or pulverised coal combustion

Lagrangian

IMPAML I strictly positive integer [IMPAMO] O L3
unit of the upstream restart file in case of Lagrangian modeling
useful if and only if ISUILA = 1

FICAML C string of 6 characters [lagamo] O L3
name of the upstream restart file in case of Lagrangian modeling. Its "format" (ASCII or binary) is automatically determined by the code.
useful if and only if ISUILA = 1

IMPMLS I strictly positive integer [IMPAMO] O L3
unit of the upstream restart file for the statistics in case of Lagrangian modeling
useful if and only if ISUIST = 1

FICMLS C string of 13 characters [lasamo] O L3
name of the upstream restart file for the statistics in case of Lagrangian modeling. Its "format" (ASCII or binary) is automatically determined by the code.
useful if and only if ISUIST = 1

IMPAVL I strictly positive integer [IMPAVA] O L3
unit of the downstream restart file in case of Lagrangian modeling
always useful in case of Lagrangian modeling

FICAVL C string of 13 characters [lagava] O L3
name of the downstream restart file in case of Lagrangian modeling
always useful in case of Lagrangian modeling

IFOAVL I 1 or 0 [IFOAVA] O L2
indicator (1: formatted, 0: binary Lagrangian downstream restart file)
always useful in case of Lagrangian modeling

IMPVLS I strictly positive integer [IMPAVA] O L3
unit of the downstream restart file for the statistics in case of Lagrangian modeling
useful in case of Lagrangian modeling with statistics

FICVLS C string of 6 characters [lasava] O L3
name of the downstream restart file for the statistics in case of Lagrangian modeling
useful in case of Lagrangian modeling with statistics

IFOVLS I 1 or 0 [IFOAVA] O L2
indicator (1: formatted, 0: binary downstream restart file for the statistics in case of Lagrangian modeling)
useful in case of Lagrangian modeling with statistics

IMPLA1 I strictly positive integer [50] O L3
unit of a file specific to Lagrangian modeling
useful in case of Lagrangian modeling

IMPLA2 I strictly positive integer [51] O L3
unit of a file specific to Lagrangian modeling
useful in case of Lagrangian modeling

IMPLA3 I strictly positive integer [52] O L3
unit of a file specific to Lagrangian modeling
useful in case of Lagrangian modeling

IMPLA4 I strictly positive integer [53] O L3
unit of a file specific to Lagrangian modeling
useful in case of Lagrangian modeling

IMPLA5 IA strictly positive integer [54 to 68] O L3
units of files specific Lagrangian modeling, 15-dimension array
useful in case of Lagrangian modeling

5.1.2 Post-processing for *EnSight* or other tools

NOTES
- The format depends on the user choices.
- The post-processing files, directly generated by the Kernel through the FVM library, can be of the following formats: *Ensight Gold*, *MED_fichier* or *CGNS*. The use of the two latter formats depends on the installation of the corresponding external libraries.
- For each quantity (problem unknow, preselected numerical variable or preselected physical parameter), the user specifies if a post-processing output is wanted. The output frequency can be set.

ICHRVL I 0 or 1 [1] O L3
indicates whether post-processing outputs are wanted (=1) or not (=0) on the 3D

volume mesh
always useful

ICHRBO I 0 or 1 [0] O L2
indicates whether post-processing outputs are wanted (=1) or not (=0) on the 2D boundary mesh
always useful

ICHRSY I 0 or 1 [0] O L2
indicates whether post-processing outputs are wanted (=1) or not (=0) on the 2D boundary mesh patches coupled with the SYRTHES conjugate heat trabsfer code
always useful

ICHRMD I 0, 1, 2, 10, 11 or 12 [0] O L2
indicates whether the post-processing geometry varies with time:
= 0: time independent
= 1: deforming or moving mesh
= 2: changing vertex coordinates and topology
= 10: time independent base, with time dependent nodal displacement field
= 11: deforming or moving mesh, plus nodal displacement field
= 12: changing vertex coordinates and topology, plus nodal displacement field

FMTCHR C string of less than 32 characters [Ensight Gold] O L1
name of the output format, among the following:
- "Ensight Gold"
- "MED_fichier" (if available)
- "CGNS" (if available)

OPTCHR C string of less than 96 characters [binary] O L2
options associated to the selected output format. The string is given as a series of key words, separated by a comma (and optional spaces). The key words are among the following:
- *text* for a text format (for *EnSight*)
- *binary* for a binary format (default choice)
- *big_endian* to force outputs to be in *big-endian* mode; this can be useful when using *ParaView*, which uses this mode by default.
- *discard_polygons* to prevent from exporting faces with more than four edges (which may not be recognised by some post-processing tools); such faces will therefore appear as "holes" in the post-processing mesh.
- *discard_polyhedra* to prevent from exporting elements which are neither tetrahedra, prisms, pyramids nor hexahedra (which may not be recognised by some post-processing tools); such elements will therefore appear as "holes" in the post-processing mesh
- *divide_polygons* to divide faces with more than four edges into triangles, so that any post-processing tool can recognise them
- *divide_polyhedra* to divide elements which are neither tetrahedra, prisms, pyramids nor hexahedra into simpler elements (tetrahedra and pyramids), so that any post-processing tool can recognise them
- *split_tensors* to export the components of a tensor variable as a series of independent variables (always the case for now)

NTCHR I -1 or strictly positive integer [-1] O L1
output period for the post-processing

= -1: only at the end of the calculation
> 0: period (every NTCHR time step)
always useful

ICHRVR IA -999, 0 or 1 [-999] O L1
for each quantity defined at the cell centers (physical or numerical variable), indicator of whether it should be post-processed or not
= -999: not initialised. By default, the post-processed quantities are the unknowns (pressure, velocity, k, ε, R_{ij}, ω, φ, $\overline{f}$, scalars), the density, the turbulent viscosity and the time step if is not uniform
= 0: not post-processed
= 1: post-processed
useful if and only if the variable is defined at the cell centers: calculation variable, physical property (time step, density, viscosity, specific heat) or turbulent viscosity if ITURB(IPHAS) $\geqslant$ 10

IPSTDV I integer $\geqslant$ 1: see below [IPSTYP*IPSTCL*IPSTFT] L1
indicates the data to post-process on the boundary mesh (the boundary mesh must have been activated with ICHRBO=1). The value of IPSTDV is the product of the following integers, depending on the variables that should be post-processed:
IPSTYP: y^+ at the boundary
IPSTCL: value of the variables at the boundary (using the boundary conditions but without reconstruction)
IPSTFT: thermal flux at the boundary ($W\,m^{-2}$), if a thermal scalar has been defined (ISCALT)
For instance, with IPSTDV=IPSTYP*IPSTCL, y^+ and the variables will be post-processed at the boundaries.
With IPSTDV=1, none of these data are post-processed at the boundaries.
always useful if ICHRBO=1

5.1.3 Chronological records of the variables on specific points

Standard use through Interface or `usini1`
For each quantity (problem unknown, preselected numerical variable or preselected physical parameter), the user indicates whether chronological records should be generated, the output period and the position of the probes. The code produces chronological records at the cell centers located closest to the geometric points defined by the user by means of their coordinates. For each quantity, the number of probes and their index-numbers must be specified (it is not mandatory to generate all the variables at all the probes).

NCAPT I positive or null integer [0] O L1
total number of probes (limited to NCAPTM=100)
always useful

XYZCAP RA real numbers [0.D0] O L1
3D-coordinates of the probes
the coordinates are written: XYZCAP(I,J), with I = 1, 2 or 3 and J $\leqslant$ NCAPT
useful if and only if NCAPT > 0

IHISVR IA -999, -1 or positive or null integer [-999] O L1
number IHISVR(N, 1) and index-numbers IHISVR(N, J>1) of the record probes to

be used for each variable, *i.e.* calculation variable or physical property defined at the cell centers. With IHISVR(N, 1)=-999 or -1, IHISVR(N, J>1) is useless.

• IHISVR(N, 1): number of record probes to use for the variable N

= -999: by default: chronogical records are generated on all the probes if N is one of the main variables (pressure, velocity, turbulence, scalars), the local time step or the turbulent viscosity. For the other quantities, no chronological record is generated.

= -1: chronological records are produced on all the probes

= 0: no chronological record on any probe

> 0: chronological record on IHISVR(N, 1) probes to be specified with IHISVR(N, J>1)

always useful, must be inferior or equal to NCAPT

• IHISVR(N, J>1): index-numbers of the probes used for the variable N (with J⩽IHISVR(N,1)+1)

= -999: by default: if IHISVR(N, 1) ≠ -999, the code stops. Otherwise, refer to the description of the case IHISVR(N, 1)=-999

useful if and only if IHISVR(N, 1) > 0

The condition IHISVR(N, J) ⩽NCAPT must be respected.

For an easier use, it is recommended to simply specify IHISVR(N,1)=-1 for all the interesting variables.

IMPHIS IA strictly positive integer [30 and 31] O L3

working units for the production of chronological record files by the Kernel

useful if and only if chronological files are produced (*i.e.* there is N for which IHISVR(N, 1) ≠ 0)

EMPHIS C string of less than 80 characters [./] O L3

directory in which the potential chronological record files generated by the Kernel will be written (path related to the execution directory)

it is recommended to keep the default value and, if necessary, to modify the launch script to copy the files in the alternate destination directory

useful if and only if chronological record files are generated (*i.e.* there is N for which IHISVR(N, 1) ≠ 0)

EXTHIS C string of less than 80 characters [hst] O L3

extension of the chronological record files

useful if and only if chronological record files are generated (*i.e.* there is N for which IHISVR(N, 1) ≠ 0)

NTHIST I -1 or strictly positive integer [1 or -1] O L1

output period of the chronological record files

= -1: no output

> 0: period (every NTHIST time step)

The default value is -1 if there is no chronological record file to generate (if there is no probe, NCAPT = 0, or if IHISVR(N, 1)=0 for all the variables) and 1 otherwise

If chronological records are generated, it is usually wise to keep the default value NTHIST=1, in order to avoid missing any high frequency evolution (unless the total number of time steps is much too big)

useful if and only if chronological record files are generated (*i.e.* there are probes (NCAPT>0) there is N for which IHISVR(N, 1) ≠ 0)

NTHSAV I -1 or positive or null integer [0] O L3

saving period the chronological record files (they are first stored in a temporary file

and then saved every NTHSAV time step)
= 0: by default (4 times during a calculation)
= -1: saving at the end of the calculation
> 0: period (every NTHSAV time step)
During the calculation, the user can read the chronological record files in the execution directory when they have been saved, *i.e.* at the first time step, at the tenth time step and when the time step number is a multiple of NTHSAV (multiple of (NTMABS-NTPABS)/4 if NTHSAV=0)
Note: using the `ficstp` *file allows to update the value of NTMABS. Hence, if the calculation is at the time step n, the saving of the chronological record files can be forced by changing NTMABS to NTPABS+4(n+1) using* `ficstp`*; after the files have been saved, NTMABS can be put back to its original value, still using* `ficstp`*.*
useful if and only if chronological record files are generated (*i.e.* there are probes (NCAPT>0) there is N for which IHISVR(N, 1) $\neq$ 0)

NON-STANDARD USE THROUGH `USHIST`
(see p.61)

IMPUSH	IA	strictly positive integer	[33 to 32+NUSHMX=49]	O	L3

units of the user chronological record files
useful if and only if the subroutine `ushist` is used

FICUSH	CA	strings of 13 characters	[ush* or ush*.n_*]	O	L2

names of the user chronological record files. In the case of a non-parallel calculation, the suffix applied the file name is a three digit number: `ush001`, `ush002`, `ush003`... In the case of a parallel-running calculation, the processor index-number is added to the suffix. For instance, for a calculation running on two processors: `ush001.n_0001`, `ush002.n_0001`, `ush003.n_0001`... and `ush001.n_0002`, `ush002.n_0002`, `ush003.n_0002`... The opening, closing, format and location of these files must be managed by the user.
useful if and only if the subroutine `ushist` is used

5.1.4 Time averages

The code allows the calculation of time averages of the type $< f_1 * f_2 ... * f_n >$. The variables f_i (defined at the cell centers) which may be taken into account are the followings:

- the solved calculation variables (velocity, pressure ...),
- the auxiliary variables from the array PROPCE (density and physical properties when they are variable in space).

The averages are treated like auxiliary variables defined at the cell centers and stored in the PROPCE array. The standard post-processing actions may therefore be activated, like the writing in the listing or the output of result files (EnSight, MED, ...). However, if the user wants to manipulate the averages in a more advanced way, it is recommended to refer first to the user subroutines `usproj` and `usvpst` which provide examples. Indeed, the PROPCE array does not contain the time averages directly, but only the cumulated value of the product $f_1 * f_2 ... * f_n$ of the selected variables f_i. The division by the cumulated duration is done only before the writing of the results. See also page 37.

To calculate p time averages of the type $< f_1 * f_2 ... * f_{n(IMOM)} >$, the user must:

- make sure that $p \leqslant$NBMOMX (do not overstep the maximum number of averages),

- make sure that $n(IMOM) \leqslant$NDGMOX for every average IMOM (do not overstep the maximum degree, *i.e* the maximum number of variables which may compose an average),

- define every average IMOM (1$\leqslant$IMOM$\leqslant$ p, without skipping any index-number) by marking out the $n(IMOM)$ variables which form it by means of the array IDFMOM(II,IMOM) (with 1$\leqslant$II$\leqslant$n(IMOM)),

- define for each average IMOM the time step number at which the calculation of the cumulated value must begin, by means of the array NTDMOM(IMOM).

The total number of averages (p=NBMOMT) is automatically determined by the code from the values of IDTMOM. The user must not specify specify it.

IDFMOM IA 0, ± variable index-number [0] O L1
Index-number of the variables composing a time average of the type $< f_1 * f_2 ... * f_n >$.
For every time average IMOM to calculate:
- if IDFMOM(II,IMOM) is positive, it refers to the index-number of a solved variable (stored in the array RTP), like for instance a velocity component (IU(IPHAS), IV(IPHAS), IW(IPHAS)) or the pressure (IPR(IPHAS))
- if IDFMOM(II,IMOM) is negative, it refers to the index-number of an auxiliary variable (stored in PROPCE), like for instance the density (IDFMOM(II,IMOM)=-IROM(IPHAS))

useful if and only if the user wants to calculate time averages

NTDMOM IA integer [-1] O L1
For every average IMOM to calculate, absolute time step number at which the calculation should begin. The value -1 means "never". Every strictly negative value (in particular -1) will considered an error and cause the calculation to stop (because the user is supposed to want to calculate the averages he has defined)
useful if and only if the user wants to calculate time averages

IMOOLD IA -2, 1$\leqslant$ integer $\leqslant$ JBMOMT [-2] O L1
Correspondence table of the averages in the case of a calculation restart. In this case, for every average IMOM in the current calculation (1$\leqslant$IMOM$\leqslant$NBMOMX), IMOOLD(IMOM) gives the index-number of the corresponding average in the previous calculation (in which JBMOMT averages were calculated).
- if IMOOLD(IMOM) = -2, the user lets the code automatically determine the correspondence. By default, the average II in the current calculation will correspond to the average II in the previous calculation, if it existed. Otherwise, II will be a new average.
- if IMOOLD(IMOM) = -1, the average is reset to zero.
- if IMOOLD(IMOM) = KK, the average IMOM will correspond to the average KK=IMOOLD(IMOM) in the previous calculation.

useful if and only if the user wants to calculate averages. Allows to add or suppress some averages, to reset them, to change their order, ...
Warning : if the calculation is not a restart, IMOOLD must not be specified (its value must remain -2)

5.1.5 Others

IMPUSR IA strictly positive integer [`70 to 69+NUSRMX=79`] O L3
unit numbers for potential user specified files
useful if and only if the user needs files (therefore always useful, by security)

FICUSR CA string of 13 characters [`usrf* or usrf*.n_*`] O L1
name of the potential user specified files. In the case of a non-parallel calculation, the suffix applied the file name is a two digit number: from `usrf01` to `usrf10`. In the case of a parallel-running calculation, the four digit processor index-number is added to the suffix. For instance, for a calculation running on two processors: from `usrf01.n_0001` to `usrf10.n_0001` and from `usrf01.n_0002` to `usrf10.n_0002`. The opening, closing, format and location of these files must be managed by the user.
useful if and only if the user needs files (therefore always useful, by security)

ILISVR IA -999, 1 or 0 [-999] O L1
for every quantity (variable, physical or numerical property ...), indicator concerning the writing in the execution report file
= -999: automatically converted into 1 if the concerned quantity is one of the main variables (pressure, velocity, turbulence, scalar), the density, the time step if IDTVAR $\neq$ 0 or the turbulent viscosity. Otherwise converted into 0.
= 1: writing in the execution listing.
= 0: no writing.
always useful

IWARNI IA integer [0] O L1
IWARNI(IVAR) characterises the level of detail of the outputs for the variable IVAR (from 1 to NVAR). The quantity of information increases with its value.
Impose the value 0 or 1 for a reasonable listing size. Impose the value 2 to get a maximum quantity of information, in case of problem during the execution.
always useful

NOMVAR CA string of less than 80 characters [“”] O L1
name of the variables (unknowns, physical properties ...): used in the execution listing, in the post-processing files, etc.
“”: not initialised (the code chooses the manes by default)
It is recommended not to define variable names of more than 8 characters, to get a clear execution listing (some advanced writing levels take into account only the first 8 characters).
always useful

NTLIST I -1 or strictly positive integer [1] O L1
writing period in the execution report file
= -1: no writing
> 0: period (every NTLIST time step)
The value of NTLIST must be adapted according to the number of iterations carried out in the calculation. Keeping NTLIST to 1 will indeed provide a maximum volume of information, but if the number of time steps is too large, the execution report file might become too big and unusable (problems with disk space, memory problems while opening the file with a text editor, problems finding the desired information in the file, ...).
always useful

NTSUIT I -1, 0 or positive or null integer [0] O L3
saving period of the restart files
= -1: only at the end of the calculation
= 0: by default (four times during the calculation)
> 0: period
always useful

5.2 Numerical options

5.2.1 Calculation management

IECAUX I 0 or 1 [1] O L2
indicates the writing (=1) or not (=0) of the auxiliary calculation restart file
always useful

ILEAUX I 0 or 1 [1] O L2
indicates the reading (=1) or not (=0) of the auxiliary calculation restart file
useful if and only if ISUITE=1

INPDT0 I 0 or 1 [0] O L1
indicates the calculation mode: 1 for a zero time step control calculation, *i.e.* without solving the transport equations, and 0 for a standard calculation.
In case of a calculation using the control mode (INPDT0=1), when the calculation is not a restart, the equations are not solved, but the physical properties and the boundary conditions are calculated. When the calculation is a restart, the physical properties and the boundary conditions are those read from the restart file (note: in the case of a second-order time scheme, the mass flow is modified as if a normal time step was realised: the mass flow generated in an potential post-processing is therefore not the mass flow read from the restart file).
In the control mode (INPDT0=1), the variable NTMABS is not used.
In the standard mode (INPDT0=0), the code solves the equations at least once, even if NTMABS=0.
always useful

ISUITE I 0 or 1 [0] C L1
indicator of a calculation restart (=1) or not (=0)
always useful

NTCABS I integer [`NTPABS`] O L3
current time step number
always useful
NTCABS is initialised and updated automatically by the code, its value is not to be modified by the user

NTMABS I integer > NTPABS [10] C L1
number of the last time step after which the calculation stops. It is an absolute number: for the restart calculations, NTMABS takes into account the number of time steps of the previous calculations. For instance, after a first calculation of 3 time steps, a restart file of 2 time steps is realised by setting NTMABS=3+2=5
always useful

NTPABS I integer [0, read] O L3
number of the last time step in the previous calculation. In the case of a restart calculation, NTPABS is read from the restart file. Otherwhise it is initialised to 0
always useful
NTPABS is initialised automatically by the code, its value is not to be modified by the user

TMARUS R -1D0 or strictly positive real [-1D0] O L3
margin in seconds on the remaining CPU time which is necessary to allow the calculation to stop automatically and write all the required results (for the machines having

a queue manager)
= -1: calculated automatically
> 0: margin defined by the user
always useful, but the default value should not be changed unless absolutely necessary.

TTCABS R positive or null real number [TTPABS] O L3
physical simulation time at the current time step. For the restart calculations, TTCABS takes into account the physical time of the previous calculations.
If the time step is uniform (IDTVAR=0 or 1), TTCABS increases of DT (value of the time step) at each iteration. If the time step is non-uniform (IDTVAR=2), TTCABS increases of DTREF at each time step.
always useful
TTCABS is initialised and updated automatically by the code, its value is not to be modified by the user

TTPABS R positive or null real number [0, read] O L3
simulation physical time at the last time step of the previous calculation. In the case of a restart calculation, TTPABS is read from the restart file. Otherwhise it is initialised to 0.
always useful
TTCABS is initialised automatically by the code, its value is not to be modified by the user

5.2.2 Scalar unknowns

ISCOLD IA -999, 1⩽ integer ⩽ JSCAL [-999] O L1
correspondence table of the scalars in the case of a calculation restart. For a calculation restart with NSCAL scalars, ISCOLD(ISCAL) gives, for every scalar ISCAL of the current calculation (1⩽ISCAL⩽NSCAL), the index-number of the corresponding scalar in the previous calculation (in which JSCAL scalars were taken into account).
ISCOLD(ISCAL) = -999: the code automatically determines the correspondence. By default, the following rules are applied:
- the user scalar II of the current calculation is initialised by the the user scalar II of the previous calculation, if this scalar existed already (otherwise, II is a new scalar).
- the particular physics scalar JJ is initialised by the particular physics scalar JJ of the previous calculation if this scalar existed already (otherwise, JJ is a new scalar).
ISCOLD(ISCAL) = KK: the scalar ISCAL (user or particular physics scalar) is initialised by the scalar KK=ISCOLD(ISCAL) of the previous calculation.
always useful. Allows to add or remove some scalars, to change the solving order, to change the physics, ...

NSCAUS I 0⩽ integer ⩽ NSCMAX [0] O L1
number of user scalars solutions of an advection equation
always useful

ISCAVR IA 0, 1 ⩽ integer ⩽ NSCAL [0] O L1
if the scalar ISCAL is the average of the square of the fluctuations of a scalar KK, then ISCAVR(ISCAL)=KK. Otherwise ISCAVR(ISCAL)=0. For ISCAL and KK, the user can only use index-numbers refering to user scalars (⩽ NSCAUS).
always useful

IPHSCA IA $1 \leqslant$ integer $\leqslant$ NPHAS [0] O L3
for every scalar ISCAL, IPHSCA(ISCAL) is the index-number of the associated phase
always useful

ISCALT IA -1 or integer > 0 [-1] O L1
for every phase IPHAS, ISCALT(IPHAS) is the index-number of the scalar representing the temperature or the enthalpy. If ISCALT(IPHAS)=-1, no scalar represents the temperature nor the enthalpy. When a specific physics module is activated (gas combustion, pulverised coal, electricity or compressible), the user must not modify ISCALT (the choice is made automatically)[35].
useful if and only if NSCAL $\geqslant 1$

ISCSTH IA -1, 0, 1, 2 or 3 [-10] O L1
type of scalar
= -10: not specified. By default, the code chooses ISCSTH(ISCAL)=0 for the scalars apart from ISCALT(IPHAS)
= -1: temperature in degrees Celsius (use only in case of radiation modeling)
= 0: passive scalar
= 1: temperature (in Kelvin if the radiation modeling is activated)
= 2: enthalpy
= 3: total energy (this value is automatically chosen by the code when using the compressible module, it must never be used otherwise and must never be specified by the user)
useful if and only if NSCAL $\geqslant 1$. The distinction between ISCSTH(ISCAL) = -1 or 1 (respectively degrees Celsius or Kelvin) is useful only in case of radiation modeling. For calculations without radiation modeling, use ISCSTH(ISCAL)=1 for the temperature. When a particular physics module is activated (gas combustion, pulverised coal, electricity or compressible), the user must not modify ISCSTH (the choice is made automatically: the solved variable is the enthalpy or the total energy).
It is also reminded that, in the case of a coupling with SYRTHES, the solved thermal variable should be the temperature (ISCSTH(ISCALT(IPHAS))=1 or -1). More precisely, everything is designed in the code to allow for the running of a calcualtion coupled with SYRTHES with the enthalpy as thermal variable (the correspondence and conversion is then specified by the user in the subroutine `usthht`). However this case has never been used in practice and has therefore not been tested. With the compressible model, it is possible to carry out calculations coupled with SYRTHES, although the thermal scalar represents the total energy and not the temperature.

ICLVFL IA -1, 0, 1 or 2 [-1] O L3
for every scalar ISCAL representing the average of the square of the fluctuations of another scalar II=ISCAVR(ISCAL) (noted f), indicator of the clipping method
= -1: no clipping because the scalar does not represent the average of the square of the fluctuations of another scalar
= 0: clipping to 0 for lower values
= 1: clipping to 0 for lower values and to $(f - f_{min})(f_{max} - f)$ for higher values, where f is the associated scalar, f_{min} and f_{max} its minimum and maximum values specified by the user (*i.e.* SCAMIN(II) and SCAMAX(II))
= 2: clipping to MAX(0,SCAMIN(ISCAL)) for lower values and to SCAMAX(ISCAL) for higher values. SCAMIN and SCAMAX are limits specified by the user
useful for the scalars ISCAL for which ISCAVR(ISCAL)>0.

[35] in the case of the compressible module, ISCALT does not correspond to the temperature nor enthalpy but to the total energy

ITBRRB I 0 or 1 [0] O L3
Reconstruction (=1) or not (=0) of the temperature, enthalpy or total energy value in the boundary cells. Useful in the case of coupling with SYRTHES and with radiation.

ICPSYR TI -999,0,1 [-999] O L3
For each scalar ISCAL, ICPSYR(ISCAL) indicates if it is coupled with SYRTHES (=1) or not (=0). There can be only one coupled scalar per calculation.
=-999: by default
• ICPSYR(ISCAL)=1 for the thermal scalar ISCAL=(ISCALT(IPHAS)) when a coupling with SYRTHES has been specified in the Interface or the launch script
• ICPSYR(ISCAL)=0 otherwise
= 0: the scalar ISCAL is not coupled with SYRTHES
= 1: the scalar ISCAL is coupled with SYRTHES
useful in case of coupling with SYRTHES

5.2.3 Definition of the equations

ISTAT IA 0 or 1 [1 or 0] O L2
for each unknown IVAR to calculate, indicates if non-stationary terms are present (ISTAT(IVAR)=1) or not (0) in the matrices.
By default, ISTAT is set to 0 for the pressure (variable IVAR=IPR(IPHAS)) or $\overline{f}$ in v2f modeling (variable IVAR=IFB(IPHAS)) and set to 1 for the other unknowns.
useful for all the unknowns

ICONV IA 0 or 1 [1 or 0] O L2
for each unknown IVAR to calculate, indicates if the convection is taken into account (ICONV(IVAR)=1) or not (0).
By default, ICONV is set to 0 for the pressure (variable IVAR=IPR(IPHAS)) or $\overline{f}$ in v2f modeling (variable IVAR=IFB(IPHAS)) and set to 1 for the other unknowns.
useful for all the unknowns

IDIFF IA 0 or 1 [1] O L2
for each unknown IVAR to calculate, indicates if the diffusion is taken into account (IDIFF(IVAR)=1) or not (0)
useful for all the unknowns

IDIFFT IA 0 or 1 [1] O L3
for each unknown IVAR to calculate, when diffusion is taken into account (IDIFF(IVAR)=1), IDIFFT(IVAR) indicates if the turbulent diffusion is taken into account (IDIFFT(IVAR)=1) or not (0)
useful for all the unknowns

IDIRCL IA 0 or 1 [1 or 0] O L3
for each unknown IVAR to calculate, indicates whether the diagonal of the matrix should be slightly shifted (IDIRCL(IVAR)=1) or not (0) if there is no Dirichlet boundary condition and if ISTAT=0. Indeed, in such a case, the matrix for the general advection/diffusion equation is singular. A slight shift in the diagonal will make it invertable again.
By default, IDIRCL is set to 1 for all the unknowns, except $\overline{f}$ in v2f modeling, since its equation contains another diagonal term that ensures the regularity of the matrix.
useful for all the unknowns

IVISSE IA 0 or 1 [1] O L3
for each phase IPHAS, indicates whether the source terms in transposed gradient and velocity divergence should be taken into account in the momentum equation. In the compressible module, these terms also account for the volume viscosity (cf. VISCV0 et IVISCV):
$\partial_i \left[(\kappa - 2/3\,(\mu + \mu_t))\partial_k U_k\right] + \partial_j \left[(\mu + \mu_t)\partial_i U_j\right]$
= 0: not taken into account
= 1: taken into account
always useful

5.2.4 Definition of the time advancement

IDTVAR I -1, 0, 1, 2 [0] O L1
type of time step
= 0: constant in time and spatially uniform
= 1: variable in time and spatially uniform
= 2: variable in time and in space
= -1: steady-state algorithm
If the numerical scheme is a second-order in time, only the option 0 is allowed.
always useful

IPTLRO I 0 or 1 [0] O L2
when density gradients and gravity are present, a local thermal time step can be calculated, based on the Brunt-Vaissala frequency. In numerical simulations, it is usually wise for the time step to be lower than this limit, otherwise numerical instabilities may appear
IPTLRO indicates whether the time step should be limited to the local thermal time step (=1) or not (=0)
when IPTLRO=1, the listing shows the number of cells where the time step has been clipped due to the thermal criterium, as well as the maximum ratio between the time step and the maximum thermal time step. If IDTVAR=0, since the time step is fixed and cannot be clipped, this ratio can be larger than 1[36]. When IDTVAR>0, this ratio will be smaller than 1, except if the constraint DTMIN has prevented the code from reaching a sufficiently low value for DT
useful when density gradients and gravity are present

CDTVAR RA strictly positive real number [1.D0] O L1
multiplicative factor applied to the time step for each scalar
Hence, the time step used when solving the evolution equation for the variable is the time step used for the dynamic equations (velocity/pressure) multiplied by CDTVAR. The size of the array CDTVAR is NVAR. For instance, the multiplicative coefficient applied to the scalar 2 is CDTVAR(ISCA(2))). Yet, the value of CDTVAR for the velocity components and the pressure is not used. Also, although it is possible to change the value of CDTVAR for the turbulent variables, it is highly unrecommended
useful if and only if NSCAL $\geqslant 1$

COUMAX R strictly positive real number [1D0] O L1
target local or maximum Courant number in case of non-constant time step
useful if IDTVAR $\neq 0$

[36] it is then the user's choice to decide whether he should diminish DTREF or not

FOUMAX R strictly positive real number [10D0] O L1
target local or maximum Fourier number in case of non-constant time step
useful if IDTVAR $\neq 0$

DTREF R strictly positive real number [-GRAND*10] C L1
reference time step
always useful.
It is the time step value used in the case of a calculation run with a uniform and constant time step, *i.e.* IDTVAR=0 (restart calculation or not). It is the value used to initialise the time step in the case of an initial calculation (ISUITE=0) run with a non-constant time step (IDTVAR=1 or 2). It is also the value used to initialise the time step in the case of a restart calculation (ISUITE=1) in which the type of time step has been changed (for instance, IDTVAR=1 in the new calculation and IDTVAR=0 or 2 in the previous calculation): see `usiniv`

DTMIN R positive or null real number [0.1D0*DTREF] O L2
lower limit for the calculated time step when non-constant time step is activated
useful if IDTVAR $\neq 0$

DTMAX R strictly positive real number [1000*DTREF] O L2
upper limit for the calculated time step when non-constant time step is activated
useful if IDTVAR $\neq 0$

VARRDT R strictly positive real number [0.1D0] O L3
maximum allowed relative increase in the calculated time step value between two succesive time steps (to ensure stability, any decrease in the time step is immediate and without limit)
useful if IDTVAR $\neq 0$

Non-constant time step
The calculation of the time step uses a reference time step DTREF (at the calculation beginning). Later, every time step, the time step value is calculated by taking into account the different existing limits, in the following order:

- COUMAX, FOUMAX: the more restrictive limit between both is used (in the compressible module, the acoustic limitation is added),
- VARRDT: progressive increase and immediate decrease in the time step,
- IPTLRO: limitation by the thermal time step,
- DTMAX and DTMIN: clipping of the time step to the maximum, then to the minimum limit.

5.2.5 Turbulence

ITURB IA 0, 10, 20, 21, 30, 31, 40, 41, 50 or 60 [-999] O L1
for each phase IPHAS, indicator of the turbulence model ITURB(IPHAS)
= -999: not initalised. This value is not allowed and must be modified by the user
= 0: laminar
= 10: mixing length (not valided)
= 20: $k-\varepsilon$
= 21: $k-\varepsilon$ with linear production (Laurence & Guimet)
= 30: $R_{ij}-\varepsilon$ "standard" LRR (Launder, Reece & Rodi)

= 31: $R_{ij} - \varepsilon$ SSG (Speziale, Sarkar & Gatski)
= 40: LES (Smagorinsky model)
= 41: LES (dynamic model)
= 50: v2-f, φ-model version
= 60: $k - \omega$, SST version
always useful

The $k - \varepsilon$ (standard and linear production) and $R_{ij} - \varepsilon$ (LRR and SSG) turbulence models implemented in *Code_Saturne* are "High-Reynolds" models. It is therefore necessary to make sure that the thickness of the first cell neighboring the wall is larger than the thickness of the viscous sublayer (at the wall, $y^+ > 2.5$ is required as a minimum, and preferably between 30 and 100)[37]. If the mesh does not respect this condition, the results may be biased (particularly if thermal processes are involved). Using scalable wall-functions (cf. key word IDEUCH) may help avoiding this problem.
The v2-f model is a "Low-Reynolds" model, it is therefore necessary to make sure that the thickness of the first cell neighboring the wall is smaller than the thickness of the viscous sublayer ($y^+ < 1$).
The $k - \omega$ SST model provides correct results whatever the thickness of the first cell. Yet, it requires the knowledge of the distance to the wall in every cell of the calculation domain. The user may refer to the key word ICDPAR for more details about the potential limitations.
The $k - \varepsilon$ model with linear production allows to correct the known flaw of the standard $k - \varepsilon$ model which overestimates the turbulence level in case of strong velocity gradients (stopping point).
With LES, the wall functions are usually not greatly adapted. It is generally more advisable (if possible) to refine the mesh towards the wall so that the first cell is in the viscous sublayer, where the boundary conditions are simple natural no-slip conditions.
Concerning the LES model, the user may refer to the subroutine `ussmag` for complements about the dynamic model. Its usage and the interpretation of its results require particular attention. In addition, the user must pay further attention when using the dynamic model with the least squares method based on a partial extended neighborhood (IMRGRA=3). Indeed, the results may be degraded if the user does not implement his own way of averaging the dynamic constant in `ussmag` (*i.e.* if the user keeps the local average based on the extended neighborhood).

IDEUCH IA 0, 1 or 2 [0 or 1] O L2
for each phase IPHAS, indicates the type of wall function is used for the velocity boundary conditions on a frictional wall.
= 0: one-scale model
= 1: two-scale model
= 2: scalable wall function
IDEUCH is initialised to 0 for ITURB(IPHAS)=0, 10, 40 or 41 (laminar, mixing length, LES).
IDEUCH is initialised to 1 for ITURB(IPHAS)=20, 21, 30, 31 or 60 ($k - \varepsilon$, $R_{ij} - \varepsilon$ LRR, $R_{ij} - \varepsilon$ SSG and $k - \omega$ SST models).
The v2f model (ITURB(IPHAS)=50) is not designed to use wall functions (the mesh must be "low Reynolds").
The value IDEUCH(IPHAS)=1 is not compatible with ITURB(IPHAS)=0, 10, 40 or 41 (laminar, mixing length and LES).
Concerning the $k - \varepsilon$ and $R_{ij} - \varepsilon$ models, the two-scales model is usually at least as satisfactory as the one-scale model.
The scalable wall function allows to virtually "shift" the wall when necessary in order to be always in a logarithmic layer. It is used to make up for the problems related to the use of High-Reynolds models on very refined meshes.
useful if ITURB(IPHAS) is different from 50

ILOGPO IA 0 or 1 [1] O L3

[37] While creating the mesh, $y^+ = \frac{yu*}{\nu}$ is generally unknown. It can be roughly estimated as $\frac{yU}{10\nu}$, where U is the characteristic velocity, ν is the kinematic viscosity of the fluid and y is the mid-height of the first cell near the wall.

for each phase IPHAS, type of wall function used for the velocity: power law (ILOGPO(IPHAS)=0) or logarithmic law (ILOGPO(IPHAS)=1)
always useful

YPLULI RA real number > 0 [1/XKAPPA,10.88D0] O L3
for each phase IPHAS, limit value of y^+ for the viscous sublayer
YPLULI depends on the chosen wall function: it is initialised to 10.88D0 for the scalable wall function (IDEUCH(IPHAS)=2), otherwise it is initialised to $1/\kappa \approx 2,38$
In LES, YPLULI is taken by default to be 10.88D0
always useful

$k-\varepsilon$, $k-\varepsilon$ WITH LINEAR PRODUCTION, V2-F AND $k-\omega$ SST

IGRAKE IA 0 or 1 [1] O L1
for each phase IPHAS, indicates if the terms related to gravity in the equations of k and ε or ω are taken into account (IGRAKE(IPHAS)=1) or not (0)
useful if and only if ITURB(IPHAS) = 20, 21, 50 or 60, (GX,GY,GZ) $\neq$ (0,0,0) and the density is not uniform

IGRHOK IA 0 or 1 [0] O L2
for each phase IPHAS, indicates if the term $\frac{2}{3}\underline{\text{grad}}\ \rho k$ is taken into account (IGRHOK(IPHAS)=1) or not (0) in the velocity equation
useful if and only if ITURB(IPHAS) = 20, 21, 50 or 60.
This term may generate non-physical velocities at the wall. When it is not explicitely taken into account, it is implicitely included into the pressure.

IKECOU IA 0 or 1 [0 or 1] O L3
for each phase IPHAS, indicates if the coupling of the source terms of k and ε or k and ω is taken into account (IKECOU(IPHAS)=1) or not (0)
if IKECOU=0 in $k-\varepsilon$ model, the term in ε in the equation of k in made implicit
IKECOU(IPHAS) is initialised to 0 if ITURB(IPHAS) = 21 or 60, and to 1 if ITURB(IPHAS)= 20
IKECOU(IPHAS)=1 is forbidden when using the v2f model (ITURB(IPHAS)=50)
useful if and only if ITURB(IPHAS) = 20, 21 or 60 ($k-\varepsilon$ and $k-\omega$ models)

RELAXK RA 0.D0 $\leqslant$ real $\leqslant$ 1.D0 [0.7D0] O L3
for each phase IPHAS, relaxation coefficient of the turbulent variables (k and ε or ω) when IKECOU(IPHAS) = 0. If IKECOU(IPHAS)=1, RELAXK is not used, whatever its value may be.
useful if and only if ITURB(IPHAS) = 20, 21, 50 or 60 and IKECOU(IPHAS)=0 ($k-\varepsilon$, v2f or $k-\omega$ models without coupling)

ICLKEP IA 0 or 1 [0] O L3
for each phase IPHAS, indicates the clipping method used for k and ε, for the $k-\varepsilon$ and v2f models
= 0: clipping in absolute value
= 1: clipping from physical relations
useful if and only if ITURB(IPHAS) = 20, 21 or 50 ($k-\varepsilon$ and v2f models). The results obtained with the method corresponding to ICLKEP(IPHAS)=1 showed in some cases a substantial sensitivity to the values of the length scale ALMAX(IPHAS).

The option ICLKEP(IPHAS)=1 is therefore not recommended, and, if chosen, must be used cautiously.

$R_{ij} - \varepsilon$ (LRR AND SSG)

ICLPTR IA 0 or 1 [0] O L3
for each phase IPHAS, indicates if R_{ij} is made partially implicit (ICLPTR(IPHAS)=1) or not (0) in the wall boundary conditions.
useful if and only if ITURB(IPHAS) = 30 or 31 ($R_{ij} - \varepsilon$ model)

ICLSYR IA 0 or 1 [0] O L3
for each phase IPHAS, indicates if R_{ij} is made partially implicit (ICLSYR(IPHAS)=1) or not (0) in the symmetry boundary conditions.
useful if and only if ITURB(IPHAS) = 30 or 31 ($R_{ij} - \varepsilon$ model)

IDIFRE IA 0 or 1 [1] O L3
for each phase IPHAS, complete (IDIFRE(IPHAS)=1) or simplified (0) taking into account of the diagonals of the diffusion tensors of R_{ij} and ε, for the LLR model.
useful if and only if ITURB(IPHAS) = 30 (LLR $R_{ij} - \varepsilon$ model)

IGRARI IA 0 or 1 [1] O L1
for each phase IPHAS, indicates if the terms related to gravity are taken into account (IGRARI(IPHAS)=1) or not (0) in the equations of $R_{ij} - \varepsilon$.
useful if and only if ITURB(IPHAS) = 30 or 31 and (GX,GY,GZ) $\neq$ (0,0,0) ($R_{ij} - \varepsilon$ model with gravity) and the density is not uniform

IRIJEC IA 0 or 1 [0] O L2
for each phase IPHAS, indicates if the wall echo terms in $R_{ij} - \varepsilon$ LRR model are taken into account (IRIJEC(IPHAS)=1) or not (0).
useful if and only if ITURB(IPHAS) = 30 ($R_{ij} - \varepsilon$ LRR).
It is not recommended to take these terms into account: they have an influence only near the walls, their expression is hardly justifiable according to some authors and, in the configurations studied with *Code_Saturne*, they did not bring any improvement in the results.
In addition, their use induces an increase in the calculation time.
The wall echo terms imply the calculation of the distance to the wall for every cell in the domain. See ICDPAR for potential restrictions due to this.

IRIJNU IA 0 or 1 [0] O L3
for each phase IPHAS, addition (IRIJNU(IPHAS)=1) or not (0) of a turbulent viscosity in the matrix of the incermental system solved for the velocity in $R_{ij} - \varepsilon$ models. The goal is to improve the stability of the calculation. The usefulness of IRIJNU(IPHAS)=1 has however not been clearly demonstrated.
Since the system is solved in incremental form, this extra turbulent viscosity does not change the final solution for steady flows. However, for unsteady flows, the parameter NSWRSM should be increased.
useful if and only if ITURB(IPHAS) = 30 or 31 ($R_{ij} - \varepsilon$ model).

IRIJRB IA 0 or 1 [0] O L3
for each phase IPHAS, reconstruction (IRIJRB(IPHAS)=1) or not (0) of the boundary

conditions at the walls for R_{ij} and ε.
useful if and only if ITURB(IPHAS) = 30 or 31 ($R_{ij} - \varepsilon$ model)

LES

IVRTEX I 0 or 1 [0] O L1
activates (=1) or not (=0) the generation of synthetic turbulence at the different inlet boundaries with the LES model (generation of unsteady synthetic eddies)
useful if ITURB(IPHAS)=40 or 41
this key word requires the completion of the routine `usvort`

ISUIVO I 0 or 1 [ISUITE] O L1
for the vortex method, indicates whether the synthetic vortices at the inlet should be initialised (=0) or read form the restart file FICMVO.
useful if ITURB(IPHAS)=40 or 41 and IVRTEX=1

IDRIES IA 0 or 1 [0,1] O L2
for each phase IPHAS, IDRIES(IPHAS) activates (1) or not (0) the van Driest wall-damping for the Smagorinsky constant (the Smagorinsky constant is multiplied by the damping function $1 - e^{-y^+/CDRIES(IPHAS)}$, where y^+ designates the adimensional distance to the nearest wall). The default value is 1 for the Smagorinsky model and 0 for the dynamic model.
the van Driest wall-damping requires the knowledge of the distance to the nearest wall for each cell in the domain. Refer to key word ICDPAR for potential limitations
useful if and only if ITURB(IPHAS) = 40 or 41

CDRIES RA real number > 0 [26.D0] O L3
for each phase IPHAS, CDRIES(IPHAS) is the constant appearing in the van Driest damping function applied to the Smagorinsky constant: $1 - e^{-y^+/CDRIES(IPHAS)}$
useful if and only if ITURB(IPHAS) = 40 or 41

CSMAGO RA real number > 0 [0.065D0] O L2
for each phase IPHAS, CSMAGO(IPHAS) is the Smagorinsky constant used in the Smagorinsky model for LES
the sub-grid scale viscosity is calculated by $\mu_{sg} = \rho C_{smago}^2 \bar{\Delta}^2 \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$ where $\bar{\Delta}$ is the width of the filter and $\bar{S}_{ij}$ the filtered strain rate
useful if and only if ITURB(IPHAS) = 40

SMAGMX RA real number > 0 [10.D0*CSMAGO] O L3
for each phase IPHAS, SMAGMX(IPHAS)**2 is the maximum allowed value for the variable C appearing in the LES dynamic model (the "square" comes from the fact that the variable of the dynamic model corresponds to the square of the constant of the Smagorinsky model). Any larger value yielded by the calculation procedure of the dynamic model will be clipped to SMAGMX(IPHAS)**2
useful if and only if ITURB(IPHAS) = 41

XLESFL RA real number > 0 [2.D0] O L3
for each phase IPHAS, XLESFL(IPHAS) is a constant used to define, for each cell Ω_i, the width of the (implicit) filter:

$\overline{\Delta} = XLESFL(IPHAS)(ALES(IPHAS) * |\Omega_i|)^{BLES(IPHAS)}$
useful if and only if ITURB(IPHAS) = 40 or 41

ALES RA real number > 0 [1.D0] O L3
for each phase IPHAS, ALES(IPHAS) is a constant used to define, for each cell Ω_i, the width of the (implicit) filter:
$\overline{\Delta} = XLESFL(IPHAS)(ALES(IPHAS) * |\Omega_i|)^{BLES(IPHAS)}$
useful if and only if ITURB(IPHAS) = 40 or 41

BLES RA real number > 0 [1.D0/3.D0] O L3
for each phase IPHAS, BLES(IPHAS) is a constant used to define, for each cell Ω_i, the width of the (implicit) filter:
$\overline{\Delta} = XLESFL(IPHAS)(ALES(IPHAS) * |\Omega_i|)^{BLES(IPHAS)}$
useful if and only if ITURB(IPHAS) = 40 or 41

XLESFD RA real number > 0 [1.5D0] O L3
for each phase IPHAS, XLESFD(IPHAS) is the constant used to define, for each cell Ω_i, the width of the explicit filter used in the framework of the LES dynamic model:
$\widetilde{\overline{\Delta}} = XLESFD(IPHAS)\overline{\Delta}$
useful if and only if ITURB(IPHAS) = 41

5.2.6 Time scheme

By default, the standard time scheme is a first-order. A second-order scheme is activated automatically with LES modeling. On the other hand, when "specific physics" (gas combustion, pulverised coal, compressible module) are activated, the second-order scheme is not allowed.

In the current version, the second-order time scheme is not compatible with the estimators (IESCAL), the velocity-pressure coupling (IPUCOU), the modeling of hydrostatic pressure (ICALHY and IPHYDR) and the time- or space-variable time step (IDTVAR).

Also, in the case of a rotation periodicity, a proper second-order is not ensured for the velocity, but calculations remain possible.

It is recommended to keep the default values of the variables listed below. Hence, in standard cases, the user does not need to specify these options.

ISCHTP IA 1 or 2 [1 or 2] O L2
for each phase IPHAS, ISCHTP(IPHAS) indicates the order of the activated time scheme (this indicator allows the code to automatically complete the other indicators related to the time scheme)
= 1: first-order
= 2: second-order
when ISCHTP(IPHAS)=2, the physical properties are by default not second-order. It it possible to modify this by means of the following indicators.
due to specific coupling between certain variables, the source terms in the turbulence equations (except convection and diffusion) cannot be second order, except with the R_{ij} models (cf. key word ISTO2T)
by default, ISCHTP(IPHAS) is initialised to 2 with the LES model and 1 otherwise
always useful

ISTMPF IA 0, 1 or 2 [0 or 1] O L3
for each phase IPHAS, ISTMPF(IPHAS) specifies the time scheme activated for the mass flow. The chosen value for ISTMPF(IPHAS) will automatically determine the

value given to the variable THETFL(IPHAS)

= 0: "explicit" first-order: the mass flow calculated at the previous time step ("n") is used in the convective terms of all the equations (momentum, turbulence and scalars

= 1: "standard" first-order: the mass flow calculated at the previous time step ("n") is used in the convective terms of the momentum equation, and the updated mass flow (time "n+1") is used in the equations of turbulence and scalars

= 2: second-order: the mass flow used in the momentum equations is extrapolated at "n+THETFL" (=n+1/2) from the values at the two former time steps (Adams Bashforth); the mass flow used in the equations for turbulence and scalars is interpolated at time "n+THETFL" (=n+1/2) from the values at the former time step and at the newly calculated "n+1" time step.

by default, ISTMPF(IPHAS)=2 is used in the case of a second-order time scheme (if ISCHTP(IPHAS)=2) and ISTMPF(IPHAS)=1 otherwise

always useful

ISNO2T IA 0, 1 or 2 [0 or 1] O L3

for each phase IPHAS, ISNO2T(IPHAS) specifies the time scheme activated for the source terms of the momentum equation, apart from convection and diffusion (for instance: head loss, transposed gradient, ...).

= 0: "standard" first-order: the terms which are linear functions of the solved variable are implicit and the others are explicit

= 1: second-order: the terms of the form $S_i\phi$ which are linear functions of the solved variable ϕ are expressed as second-order terms by interpolation (according to the formula $(S_i\phi)^{n+\theta} = S_i^n[(1-\theta)\phi^n + \theta\phi^{n+1}]$, θ being given by the value of THETAV associated with the variable ϕ) ; the other terms S_e are expressed as second-order terms by extrapolation (according to the formula $(S_e)^{n+\theta} = [(1+\theta)S_e^n - \theta S_e^{n-1}]$, θ being given by the value of THETSN(IPHAS)=0.5D0)

= 2: the linear terms $S_i\phi$ are treated in the same way as when ISNO2T=1; the other terms S_e are extrapolated according to the same formula as when ISNO2T=1, but with θ=THETSN(IPHAS)=1.D0

by default, ISNO2T(IPHAS) is initialised to 1 (second-order) when the selected time scheme is second-order (ISCHTP=2), otherwise to 0.

always useful

ISTO2T IA 0, 1 or 2 [0] O L3

for each phase IPHAS, ISTO2T(IPHAS) specifies the time scheme activated for the source terms of the turbulence equations (related to k, R_{ij}, ε, ω, φ, $\overline{f}$), apart from convection and diffusion.

= 0: "standard" first-order: the terms which are linear functions of the solved variable are implicit and the others are explicit

= 1: second-order: the terms of the form $S_i\phi$ which are linear functions of the solved variable ϕ are expressed as second-order terms by interpolation (according to the formula $(S_i\phi)^{n+\theta} = S_i^n[(1-\theta)\phi^n + \theta\phi^{n+1}]$, θ being given by the value of THETAV associated with the variable ϕ) ; the other terms S_e are expressed as second-order terms by extrapolation (according to the formula $(S_e)^{n+\theta} = [(1+\theta)S_e^n - \theta S_e^{n-1}]$, θ being given by the value of THETST(IPHAS)=0.5D0)

= 2: the linear terms $S_i\phi$ are treated in the same way as when ISTO2T=1; the other terms S_e are extrapolated according to the same formula as when ISTO2T=1, but with θ=THETST(IPHAS)=1.D0

due to certain specific couplings between the turbulence equations, ISTO2T(IPHAS) is allowed the value 1 or 2 only for the R_{ij} models (ITURB(IPHAS)=30 or 31); hence, it is always initialised to 0.

always useful

ISSO2T IA 0, 1 or 2 [0 or 1] O L3
for each scalar ISCAL, ISSO2T(ISCAL) specifies the time scheme activated for the source terms of the equation for the scalar, apart from convection and diffusion (for instance: variance production, user-specified terms, ...).
= 0: "standard" first-order: the terms which are linear functions of the solved variable are implicit and the others are explicit
= 1: second-order: the terms of the form $S_i\phi$ which are linear functions of the solved variable ϕ are expressed as second-order terms by interpolation (according to the formula $(S_i\phi)^{n+\theta} = S_i^n[(1-\theta)\phi^n + \theta\phi^{n+1}]$, θ being given by the value of THETAV associated with the variable ϕ) ; the other terms S_e are expressed as second-order terms by extrapolation (according to the formula $(S_e)^{n+\theta} = [(1+\theta)S_e^n - \theta S_e^{n-1}]$, θ being given by the value of THETSS(ISCAL)=0.5D0)
= 2: the linear terms $S_i\phi$ are treated in the same way as when ISSO2T=1; the other terms S_e are extrapolated according to the same formula as when ISSO2T=1, but with θ=THETSS(ISCAL)=1.D0
by default, ISSO2T(ISCAL) is initialised to 1 (second-order) when the selected time scheme is second-order (ISCHTP=2), otherwise to 0.
always useful

IROEXT IA 0, 1 or 2 [0] O L3
for each phase IPHAS, IROEXT(IPHAS) specifies the time scheme activated for the physical property ϕ "density".
= 0: "standard" first-order: the value calculated at the beginning of the current time step (from the variables known at the end of the previous time step) is used
= 1: second-order: the physical property ϕ is extrapolated according to the formula $\phi^{n+\theta} = [(1+\theta)\phi^n - \theta\phi^{n-1}]$, θ being given by the value of THETRO(IPHAS)=0.5D0
= 2: first-order: the physical property ϕ is extrapolated at $n+1$ according to the same formula as when IROEXT=1 but with θ=THETRO(IPHAS)=1.D0
always useful

IVIEXT IA 0, 1 or 2 [0] O L3
for each phase IPHAS, IVIEXT(IPHAS) specifies the time scheme activated for the physical property ϕ "total viscosity" (molecular+turbulent or sub-grid viscosities).
= 0: "standard" first-order: the value calculated at the beginning of the current time step (from the variables known at the end of the previous time step) is used
= 1: second-order: the physical property ϕ is extrapolated according to the formula $\phi^{n+\theta} = [(1+\theta)\phi^n - \theta\phi^{n-1}]$, θ being given by the value of THETVI(IPHAS)=0.5D0
= 2: first-order: the physical property ϕ is extrapolated at $n+1$ according to the same formula as when IVIEXT=1, but with θ=THETVI(IPHAS)=1.D0
always useful

ICPEXT IA 0, 1 or 2 [0] O L3
for each phase IPHAS, ICPEXT(IPHAS) specifies the time scheme activated for the physical property ϕ "specific heat".
= 0: "standard" first-order: the value calculated at the beginning of the current time step (from the variables known at the end of the previous time step) is used
= 1: second-order: the physical property ϕ is extrapolated according to the formula $\phi^{n+\theta} = [(1+\theta)\phi^n - \theta\phi^{n-1}]$, θ being given by the value of THETCP(IPHAS)=0.5D0
= 2: first-order: the physical property ϕ is extrapolated at $n+1$ according to the same formula as when ICPEXT=1, but with θ=THETCP(IPHAS)=1.D0
always useful

IVSEXT IA 0, 1 ou 2 [0] O L3
for each scalar ISCAL, IVSEXT(ISCAL) specifies the time scheme activated for the

physical property ϕ "diffusivity".
= 0: "standard" first-order: the value calculated at the beginning of the current time step (from the variables known at the end of the previous time step) is used
= 1: second-order: the physical property ϕ is extrapolated according to the formula $\phi^{n+\theta} = [(1+\theta)\phi^n - \theta\phi^{n-1}]$, θ being given by the value of THETVS(ISCAL)=0.5D0
= 2: first-order: the physical property ϕ is extrapolated at $n+1$ according to the same formula as when IVSEXT=1, but with θ=THETVS(ISCAL)=1.D0
always useful

THETAV RA 0.D0 $\leqslant$ real $\leqslant$1.D0 [1.D0 or 0.5D0] O L3
for each variable IVAR, THETAV(IVAR) is the value of θ used to express at the second-order the terms of convection, diffusion and the source terms which are linear functions of the solved variable (according to the formula $\phi^{n+\theta} = (1-\theta)\phi^n + \theta\phi^{n+1}$). Generally, only the values 1.0D0 and 0.5D0 are used. The user is not allowed to modify this variable.
= 1.D0: first-order
= 0.5D0: second-order
Concerning the pressure, the value of THETAV is always 1.0D0. Concerning the other variables, the value THETAV=0.5D0 is used when the second-order time scheme is activated by ISCHTP=2 (standard value for LES calculations), otherwise THETAV is set to 1.0D0.
always useful

THETFL RA 0.D0 $\leqslant$ real $\leqslant$1.D0 [0.D0 or 0.5D0] O L3
for each phase IPHAS, THETFL(IPHAS) is the value of θ used to interpolate the convective fluxes of the variables when a second-order time scheme has been activated for the mass flow (see ISTMPF)
generally, only the value 0.5D0 is used. The user is not allowed to modify this variable.
= 0.0D0: "explicit" first-order (corresponds to ISTMPF(IPHAS)=0 or 1)
= 0.5D0: second-order (corresponds to ISTMPF(IPHAS)=2). The mass flux will be interpolated according to the formula $Q^{n+\theta} = \frac{1}{2-\theta}Q^{n+1} + \frac{1-\theta}{2-\theta}Q^{n+1-\theta}$).
always useful

THETSN RA 0.D0 $\leqslant$ real $\leqslant$1.D0 [0.0D0, 0.5D0 or 1.D0] O L3
for each phase IPHAS, THETSN(IPHAS) is the value of θ used to extrapolate the non linear explicit source terms S_e of the momentum equation, when the source term extrapolation has been activated (see ISNO2T), following the formula
$(S_e)^{n+\theta} = (1+\theta)S_e^n - \theta S_e^{n-1}$
the value of θ=THETSN(IPHAS) is deduced from the value chosen for ISNO2T(IPHAS). Generally, only the value 0.5D0 is used. The user is not allowed to modify this variable.
= 0.0D0: first-order (unused, corresponds to ISNO2T(IPHAS)=0)
= 0.5D0: second-order (used when ISNO2T(IPHAS)=1)
= 1.0D0: first-order (used when ISNO2T(IPHAS)=2)
always useful

THETST RA 0.D0 $\leqslant$ real $\leqslant$1.D0 [0.0D0, 0.5D0 or 1.D0] O L3
for each phase IPHAS, THETST(IPHAS) is the value of θ used to extrapolate the non linear explicit source terms S_e of the turbulence equations, when the source term extrapolation has been activated (see ISTO2T), following the formula
$(S_e)^{n+\theta} = (1+\theta)S_e^n - \theta S_e^{n-1}$
the value of θ=THETSN(IPHAS) is deduced from the value chosen for ISTO2T(IPHAS). Generally, only the value 0.5D0 is used. The user is not allowed to modify this variable.

= 0.0D0: first-order (unused, corresponds to ISTO2T(IPHAS)=0)
= 0.5D0: second-order (used when ISTO2T(IPHAS)=1)
= 1.0D0: first-order (used when ISTO2T(IPHAS)=2)
always useful

THETSS RA 0.D0 ⩽ real ⩽1.D0 [0.0D0, 0.5D0 or 1.D0] O L3
for each scalar ISCAL, THETSS(ISCAL) is the value of θ used to extrapolate the non linear explicit source terms S_e of the scalar equation, when the source term extrapolation has been activated (see ISSO2T), following the formula
$(S_e)^{n+\theta} = (1+\theta)S_e^n - \theta S_e^{n-1}$
the value of θ=THETSS(ISCAL) is deduced from the value chosen for ISSO2T(ISCAL). Generally, only the value 0.5D0 is used. The user is not allowed to modify this variable.
= 0.0D0: first-order (unused, corresponds to ISSO2T(ISCAL)=0)
= 0.5D0: second-order (used when ISSO2T(ISCAL)=1)
= 1.0D0: first-order (used when ISSO2T(ISCAL)=2)
useful if NSCAL>1

THETRO RA 0.D0 ⩽ real ⩽1.D0 [0.0D0, 0.5D0 or 1.D0] O L3
for each phase IPHAS, THETRO(IPHAS) is the value of θ used to extrapolate the physical property ϕ "density" when the extrapolation has been activated (see IROEXT),according to the formula $\phi^{n+\theta} = (1+\theta)\phi^n - \theta\phi^{n-1}$
the value of θ=THETRO(IPHAS) is deduced from the value chosen for IROEXT(IPHAS). Generally, only the value 0.5D0 is used. The user is not allowed to modify this variable.
= 0.0D0: first-order (unused, corresponds to IROEXT(IPHAS)=0)
= 0.5D0: second-order (corresponds to IROEXT(IPHAS)=1)
= 1.0D0: first-order (corresponds to IROEXT(IPHAS)=2)
always useful

THETVI RA 0.D0 ⩽ real ⩽1.D0 [0.0D0, 0.5D0 or 1.D0] O L3
for each phase IPHAS, THETVI(IPHAS) is the value of θ used to extrapolate the physical property ϕ "total viscosity" when the extrapolation has been activated (see IVIEXT),according to the formula $\phi^{n+\theta} = (1+\theta)\phi^n - \theta\phi^{n-1}$
the value of θ=THETVI(IPHAS) is deduced from the value chosen for IVIEXT(IPHAS). Generally, only the value 0.5D0 is used. The user is not allowed to modify this variable.
= 0.0D0: first-order (unused, corresponds to IVIEXT(IPHAS)=0)
= 0.5D0: second-order (corresponds to IVIEXT(IPHAS)=1)
= 1.0D0: first-order (corresponds to IVIEXT(IPHAS)=2)
always useful

THETCP RA 0.D0 ⩽ real ⩽1.D0 [0.0D0, 0.5D0 or 1.D0] O L3
for each phase IPHAS, THETCP(IPHAS) is the value of θ used to extrapolate the physical property ϕ "specific heat" when the extrapolation has been activated (see ICPEXT),according to the formula $\phi^{n+\theta} = (1+\theta)\phi^n - \theta\phi^{n-1}$
the value of θ=THETCP(IPHAS) is deduced from the value chosen for ICPEXT(IPHAS). Generally, only the value 0.5D0 is used. The user is not allowed to modify this variable.
= 0.0D0: first-order (unused, corresponds to ICPEXT(IPHAS)=0)
= 0.5D0: second-order (corresponds to ICPEXT(IPHAS)=1)
= 1.0D0: first-order (corresponds to ICPEXT(IPHAS)=2)
always useful

THETVS RA 0.D0 ⩽ real ⩽1.D0 [0.0D0, 0.5D0 or 1.D0] O L3
for each scalar ISCAL, THETVS(ISCAL) is the value of θ used to extrapolate the physical property ϕ "diffusivity" when the extrapolation has been activated (see IVSEXT),according to the formula $\phi^{n+\theta} = (1+\theta)\phi^n - \theta\phi^{n-1}$
the value of θ=THETVS(ISCAL) is deduced from the value chosen for IVSEXT(ISCAL). Generally, only the value 0.5D0 is used. The user is not allowed to modify this variable.
= 0.0D0: first-order (unused, corresponds to IVSEXT(ISCAL)=0)
= 0.5D0: second-order (corresponds to IVSEXT(ISCAL)=1)
= 1.0D0: first-order (corresponds to IVSEXT(ISCAL)=2)
useful if NSCAL>1

5.2.7 Gradient reconstruction

IMRGRA I 0, 1, 2, 3 or 4 [0] O L2
indicates the type of gradient reconstruction (one method for all the variables)
= 0: iterative reconstruction of the non-orthogonalities
= 1: least squares method based on the first neighbor cells (cells which share a face with the treated cell)
= 2: least squares method based on the extended neighborhood (cells which share a node with the treated cell)
= 3: least squares method based on a partial extended neighborhood (all first neighbors plus the extended neighborhood cells that are connected to a face where the non-orthogonality angle is larger than parameter ANOMAX)
= 4: iterative reconstruction with initialisation using the least squares method (first neighbors)
if IMRGRA fails due to probable mesh quality problems, it is usually effective to use IMRGRA=3. Moreover, IMRGRA=3 is usually faster than IMRGRA=0 (but with less feedback on its use).
it should be noted that IMRGRA=1, 2 or 3 automatically triggers a gradient limitation procedure. See IMLIGR.
useful if and only if there is N so that NSWRGR(N) > 1

NSWRGR IA positive integer [100] O L3
for each unknown IVAR, NSWRGR(IVAR) ⩽ 1 indicates that the gradients are not reconstructed
if IMRGRA = 0 or 4, NSWRGR(IVAR) is the number of iterations for the gradient reconstruction
if IMRGRA = 1, 2 or 3, NSWRGR(IVAR) > 1 indicates that the gradients are reconstructed (but the method is not iterative, so any value larger than 1 for NSWRGR yields the same result)
useful for all the unknowns

EPSRGR RA real number > 0 [1.D-5] O L3
for each unknown IVAR, relative precision for the iterative gradient reconstruction: EPSRGR(IVAR)
useful for all the unknowns when IMRGRA = 0 or 4

IMLIGR IA -1, 0 or 1 [-1 or 1] O L3
for each unknown IVAR, indicates the type of gradient limitation: IMLIGR(IVAR)
=-1: no limitation
= 0: based on the neighbors

= 1: superior order
for all the unknowns, IMLIGR is initialised to -1 if IMRGRA=0 or 4 and to 1 if IMRGRA = 1, 2 or 3
useful for all the unknowns

CLIMGR RA real number > 0 [1.5D0] O L3
for each unknown IVAR, factor of gradient limitation: CLIMGR(IVAR) (high value means little limitation)
useful for all the unknowns IVAR for which IMLIGR(IVAR) ≠ -1

EXTRAG RA 0.D0, 0.5D0 or 1.D0 [0.D0] O L3
for the variable "pressure" IVAR=IPR(IPHAS), extrapolation coefficient of the gradients at the boundaries. It affects only the Neumann conditions. The only possible values of EXTRAG(IPR(IPHAS)) are:
= 0.D0: homogeneous Neumann calculated at first-order
= 0.5D0: improved homogeneous Neumann, calculated at second-order in the case of an orthogonal mesh and at first-order otherwise
= 1.D0: gradient extrapolation (gradient at the boundary face equal to the gradient in the neighbor cell), calculated at second-order in the case of an orthogonal mesh and at first-order otherwise
EXTRAG often allows to correct the non-physical velocities that appear on horizontal walls when density is variable and there is gravity. It is strongly advised to keep EXTRAG=0 for the variables apart from pressure. See also IPHYDR.
In practice, only the values 0.D0 and 1.D0 are allowed. The value 0.5D0 isn't allowed by default (but the lock can be overridden if necessary, contact the development team).
always useful

ANOMAX R 0.D0 ⩽ real ⩽ $\pi/2$ [$\pi/4$] O L3
limit non-orthogonality angle used to restrict the extended neighborhood for the gradient calculation with IMRGRA=3.
ANOMAX=0 will yield the same result as IMRGRA=2 (full extended neighborhood).
ANOMAX=$\pi/2$ will yield the same result as IMRGRA=2 (first neighbors only)[38]
useful if and only if IMRGRA=3

5.2.8 Solution of the linear systems

IRESOL IA -1, 1000*IPOL+J [-1] O L3
for each unknown IVAR, IRESOL(IVAR) indicates the method used for the solution of the linear system
= -1: automatically managed by the code (conjugate gradient for the pressure IVAR=IPR(IPHAS) or any variable which is not convected, Jacobi for the others. Diagonal preconditioning with conjugate gradient).
= IPOL*1000+J with J= 0: conjugate gradient
J= 1: Jacobi
J= 2: stabilised bi-conjugate gradient (BI-CGSTAB)
IPOL is the degree of the Neumann polynomial used for the preconditioning[39].

[38] except for pathological cases where the non-orthogonality angle of a face would be larger than $\pi/2$

[39] D being the diagonal part of A and X its extra-diagonal part, it can be written $A = D(Id + D^{-1}X)$. Therefore $A^{-1} = (Id + D^{-1}X)^{-1}D^{-1}$. A series development of $Id + D^{-1}X$ can then be used which yields, symbolically, $Id + \sum_{I=1}^{IPOL} (-D^{-1}X)^I$.

IPOL is necessarily null with the Jacobi algorithm.
Concerning the computational time, the performance depends on the case. If a preconditioning method different from the diagonal preconditioning is to be used, it seems to be better to restrict to a first-order preconditioning (IPOL=1). This preconditioning may save up to 10% of time in some cases but in the others it may also increase the computational time by a few percents
always useful

NITMAX IA integer > 0 [10000] O L3
for each unknown IVAR, maximum number of iterations for the solution of the linear systems: NITMAX(IVAR)
when the algebraic multigrid option is activated for the variable IVAR (IMGR(IVAR)=1), NITMAX(IVAR) is the maximum number of iterations for the solution on the coarsest mesh
always useful

EPSILO RA real number > 0 [1.D-8,1.D-5] O L3
for each unknown IVAR, relative precision for the solution of the linear system. The default value is EPSILO(IVAR)=1.D-8. This value is set low on purpose. When there are enough iterations on the reconstruction of the right-hand side of the equation, the value may be increased (by default, in case of second-order in time, with NSWRSM = 5 or 10, EPSILO is increased to 1.D-5).
always useful

IMGR IA 0 or 1 [0] O L3
for each unknown IVAR, indicates the use (IMGR(IVAR)=1) or not (=0) of the algebraic multigrid method for the solution of the linear systems
IMGR(IVAR) can be set independently for every variable
always useful. Generally, its use is designed for the variable "pressure" in case of meshes with strongly stretched cells. It is recommended not to modify IMGR

NCEGRM I integer > 0 [30] O L3
for the multigrid method, maximum number of cells on the coarsest grid
useful if and only if IMGR(IVAR) = 1 for at least one variable IVAR

NCYMAX IA integer > 0 [100] O L3
for each unknown IVAR, NCYMAX(IVAR) is the maximum number of cycles when using the multigrid method.
useful if and only if IMGR(IVAR) = 1

NGRMAX I 1⩽ integer ⩽NGRMMX [NGRMMX] O L3
when using the multigrid method, maximum number of grid levels
useful if and only if IMGR(IVAR) = 1 for at least one variable IVAR

NITMGF IA integer > 0 [10] O L3
for each unknown IVAR, NITMGF(IVAR) is the maximum number of iterations on the intermediary grids when the multigrid method is used
useful if and only if IMGR(IVAR) = 1

Warning
The algebraic multigrid method does not work when the mesh contains subdivided faces (or more generally when two different faces have the same pair of neighbors). In addition, it has been validated up to now only for the variable "pressure" (IMGR(IPR(IPHAS))=1) and with non-parallel computations.

5.2.9 Convective scheme

BLENCV RA $0 \leqslant$ real $\leqslant 1$ [0.D0 or 1.D0] O L1
for each unknown IVAR to calculate, BLENCV(IVAR) indicates the proportion of second-order convective scheme (0.D0 corresponds to an "upwind" first-order scheme) ; in case of LES calculation, a second-order scheme is recommended and activated by default (BLENCV=1.D0)
useful for all the unknowns IVAR for which ICONV(IVAR) = 1

ISCHCV IA 0 or 1 [1] O L2
for each unknown IVAR to calculate, ISCHCV(IVAR) indicates the type of second-order convective scheme
= 0: Second Order Linear Upwind
= 1: Centered
useful for all the unknowns IVAR which are convected (ICONV(IVAR)=1) and for which a second-order scheme is used (BLENCV(IVAR) > 0)

ISSTPC IA 0 or 1 [0] O L2
for each unknown IVAR to calculate, ISSTPC(IVAR) indicates whether a "slope test" should be used to switch from a second-order to an "upwind" convective scheme under certain conditions, to ensure stability.
= 0: "slope test" activated for the considered unknown
= 1: "slope test" deactivated for the considered unknown
useful for all the unknowns IVAR which are convected (ICONV(IVAR)=1) and for which a second-order scheme is used (BLENCV(IVAR) > 0).
the use of the "slope test" stabilises the calculation but may bring the order in space to decrease quickly.

5.2.10 Pressure-continuity step

IPRCO I 0 or 1 [1] O L3
indicates if the pressure-continuity step is taken into account (1) or not (0)
always useful

ARAK RA $0 <$ real $\leqslant 1$ [1.D0] O L3
for each phase IPHAS, ARAK(IPHAS) is the Arakawa coefficient before the Rhie& Chow filter
always useful

RELAXP RA $0 <$ real $\leqslant 1$ [1.D0] O L2
for each phase IPHAS, relaxation of the pressure increment during the solution of the system (RELAXP(IPHAS)=1: no relaxation)
can improve the convergence in case of meshes of insufficient quality
always useful

IREVMC IA 0, 1 or 2 [0] O L3
for each phase IPHAS, method used to update the velocity after the pressure correction:
- standard gradient of pressure increment (IREVMC(IPHAS)=0)
- least squares on the pressure increment (IREVMC(IPHAS)=1)
-"RT0" *i.e.* least squares on the updated mass flux (IREVMC(IPHAS)=2)

the method IREVMC(IPHAS)=2 is generally not recommended
always useful

IPHYDR I 0 or 1 [0] O L2
method for taking into account the balance between the pressure gradient and the source terms (gravity and head losses): by extension it will be referenced as "taking into account of the hydrostatic pressure"
= 0: standard algorithm
= 1: improved algorithm
always useful
When the density effects are important, the choice of IPHYDR=1 allows to improve the interpolation of the pressure and correct the non-physical velocities which may appear in highly stratified areas or near horizontal walls (thus avoiding the use of EXTRAG if the non-physical velocities are due only to gravity effects).
The improved algorithm also allows to eradicate the velocity oscillations which tend to appear at the frontiers of areas with high head losses.
In the case of a stratified flow, the calculation cost is higher when the improved algorithm is used (about 30% depending on the case) because the hydrostatic pressure has to be recalculated at the outlet boundary conditions: see ICALHY.
On meshes of insufficient quality, in order to improve the convergence, it may be useful to increase the number of iterations for the reconstruction of the pressure right-hand member, *i.e.* NSWRSM(IPR(IPHAS)).
If head losses are present just along an outlet boundary, it is necessary to specify ICALHY=0 in order to deactivate the recalculation of the hydrostatic pressure at the boundary, which may otherwise cause instabilities.

ICALHY I 0 or 1 [0 or 1] O L3
activates the calculation of hydrostatic pressure boundary conditions at outlet boundaries
= 0: no calculation of the hydrostatic pressure at the outlet boundary
= 1: calculation of the hydrostatic pressure at the outlet boundary
always useful
This option is automatically specified depending on the choice of IPHYDR and the value of gravity (ICALHY=1 if IPHYDR=1 and gravity is different from 0; otherwise ICALHY=0). The activation of this option generates an additional calculation cost (about 30% depending on the case).
If head losses are present just along an outlet boundary, it is necessary to specify ICALHY=0 in order to deactivate the recalculation of the hydrostatic pressure at the boundary, which may otherwise cause instabilities

5.2.11 Error estimators for Navier-Stokes

There are currently NESTMX=4 types of local estimators provided at every time step, with two possible definitions for each[40]. These scalars indicate the areas (cells) in which some error types may be important. They are stored in the array PROPCE containing the properties at the cells (see IESTIM). For each estimator, the code writes the minimum and maximum values in the listing and generates post-processing outputs along with the other variables.

The additional memory cost is about one real number per cell and per estimator. The additional calculation cost is variable. For instance, on a simple test case, the total estimator IESTOT generates an additional cost of 15 to 20 % on the CPU time[41] ; the cost of the three others may be neglected. If

[40] choice made by the user
[41] indeed, all the first-order in space differential terms have to be recalculated at the time t^{n+1}

the user wants to avoid the calculation of the estimators during the computation, it is possible to run a calculation without estimators first, and then activate them on a restart of one or two time steps.

It is recommended to use the estimators only for visual and qualitative analysis. Also, their use is compatible neither with a second-order time scheme nor with a calculation with a frozen velocity field.

IEST = IESPRE: prediction (default name: EsPre). After the velocity prediction step (yielding $\underline{u}^*$), the estimator $\eta_{i,k}^{pred}(\underline{u}^*)$, local variable calculated at every cell Ω_i, is created from $\underline{\mathcal{R}}^{pred}(\underline{u}^*)$, which represents the residual of the equation solved during this step:

$$\begin{aligned}\underline{\mathcal{R}}^{pred}(\underline{u}^*) &= \rho^n \frac{\underline{u}^* - \underline{u}^n}{\Delta t} + \rho^n \underline{u}^n \cdot \underline{\underline{grad}}(\underline{u}^*) - div\left((\mu+\mu_t)^n \underline{\underline{grad}}(\underline{u}^*)\right) + \underline{\text{grad}}\ (P^n) \\ &- \text{ rest of the right-hand member } (\underline{u}^n, P^n, \text{other variables}^n)\end{aligned}$$

By definition:

$$\eta_{i,k}^{pred}(\underline{u}^*) = |\Omega_i|^{(k-2)/2}\ ||\underline{\mathcal{R}}^{pred}(\underline{u}^*)||_{I\!L^2(\Omega_i)}$$

• The first family, $k = 1$, suppresses the volume $|\Omega_i|$ which intrinsicly appears with the norm $I\!L^2(\Omega_i)$.

• The second family, $k = 2$, exactly represents the norm $I\!L^2(\Omega_i)$. The size of the cell therefore appears in its calculation and induces a weighting effect.

$\eta_{i,k}^{pred}(\underline{u}^*)$ is ideally equal to zero when the reconstruction methods are perfect and the associated system is solved exactly.

IEST = IESDER: drift (default name: EsDer). The estimator $\eta_{i,k}^{der}(\underline{u}^{n+1})$ is based on the following quantity (intrinsic to the code):

$$\begin{aligned}\eta_{i,k}^{der}(\underline{u}^{n+1}) &= |\Omega_i|^{(k-2)/2} ||div(\text{corrected mass flow after the pressure step}) - \ \Gamma||_{L^2(\Omega_i)} \\ &= |\Omega_i|^{(1-k)/2} |div(\text{corrected mass flow after the pressure step}) - \ \Gamma|\end{aligned} \qquad (3)$$

Ideally, it is equal to zero when the Poisson equation related to the pressure is solved exactly.

IEST = IESCOR: correction (default name: EsCor). The estimator $\eta_{i,k}^{corr}(\underline{u}^{n+1})$ comes directly from the mass flow calculated with the updated velocity field:

$$\eta_{i,k}^{corr}(\underline{u}^{n+1}) = |\Omega_i|^{\delta_{2,k}}\ |div(\rho^n \underline{u}^{n+1}) - \ \Gamma|$$

The velocities $\underline{u}^{n+1}$ are taken at the cell centers, the divergence is calculated after projection on the faces.

$\delta_{2,k}$ represents the Kronecker symbol.

• The first family, $k = 1$, is the absolute raw value of the divergence of the mass flow minus the mass source term.

• The second family, $k = 2$, represents a physical property and allows to evaluate the difference in $kg.s^{-1}$.

Ideally, it is equal to zero when the Poisson equation is solved exactly and the projection from the mass flux at the faces to the velocity at the cell centers is made in a set of functions with null divergence.

IEST = IESTOT: total (default name: EsTot). The estimator $\eta_{i,k}^{tot}(\underline{u}^{n+1})$, local variable calculated at every cell Ω_i, is based on the quantity $\underline{\mathcal{R}}^{tot}(\underline{u}^{n+1})$, which represents the residual of the equation using the updated values of $\underline{u}$ and P:

$$\begin{aligned}\underline{\mathcal{R}}^{tot}(\underline{u}^{n+1}) &= \rho^n \frac{\underline{u}^{n+1} - \underline{u}^n}{\Delta t} + \rho^n \underline{u}^{n+1} \cdot \underline{\underline{grad}}(\underline{u}^{n+1}) - div\left((\mu+\mu_t)^n \underline{\underline{grad}}(\underline{u}^{n+1})\right) + \underline{\text{grad}}\ (P^{n+1}) \\ &- \text{ rest of the right-hand member } (\underline{u}^{n+1}, P^{n+1}, \text{other variables}^n)\end{aligned}$$

By definition:

$$\eta_{i,k}^{tot}(\underline{u}^{n+1}) = |\Omega_i|^{(k-2)/2}\ ||\underline{\mathcal{R}}^{tot}(\underline{u}^{n+1})||_{I\!L^2(\Omega_i)}$$

The mass flux in the convective term is recalculated from $\underline{u}^{n+1}$ expressed at the cell centers (and not taken from the updated mass flow at the faces).

As for the prediction estimator:

• The first family, $k = 1$, suppresses the volume $|\Omega_i|$ which intrinsicly appears with the norm $I\!L^2(\Omega_i)$.

• The second family, $k = 2$, exactly represents the norm $I\!L^2(\Omega_i)$. The size of the cell therefore appears in its calculation and induces a weighting effect.

The estimators are evaluated depending on the values of IESCAL.

IESCAL IA 0, 1 or 2 [0] O L1
for each phase IPHAS, IESCAL(IEST,IPHAS) indicates the calculation mode for the error estimator IEST (IESPRE, IESDER, IESCOR or IESTOT), for the Navier-Stokes equation:
IESCAL = 0: estimator not calculated,
IESCAL = 1: the estimator $\eta^*_{i,1}$ is calculated, without contribution of the volume,
IESCAL = 2: the estimator $\eta^*_{i,2}$ is calculated, with contribution of the volume ("norm L^2"), except for IESCOR, for which $|\Omega_i|\ \eta^{corr}_{i,1}$ is calculated.

The name of the estimators appearing in the listing and the post-processing is made up of the default name (given before), followed first by the value of IESCAL, then by the phase number. For instance, EsPre201 is the estimator IESPRE calculated with IESCAL=2 for the phase 01.
always useful

5.2.12 Calculation of the distance to the wall

ICDPAR I -1, 1, -2 or 2 [-1] O L2
specifies the method used to calculate the distance to the wall y and the adimensional distance y^+ for all the cells of the calculation domain (when necessary):
= 1: standard algorithm (based on a Poisson equation for y and convection equation for y^+), with reading of the distance to the wall from the restart file if possible
=-1: standard algorithm (based on a Poisson equation for y and convection equation for y^+), with systematic recalculation of the distance to the wall in case of calculation restart
= 2: former algorithm (based on geometrical considerations), with reading of the distance to the wall from the restart file if possible
=-2: former algorithm (based on geometrical considerations) with systematic recalculation of the distance to the wall in case of calculation restart
In case of restart calculation, if the position of the walls haven't changed, reading the distance to the wall from the restart file can save a fair amount of CPU time.
Useful in $R_{ij} - \varepsilon$ model with wall echo (ITURB(IPHAS)=30 and IRIJEC=1), in LES with van Driest damping (ITURB(IPHAS)=40 and IDRIES(IPHAS)=1) and in $k-\omega$ SST (ITURB(IPHAS)=60).
By default, ICDPAR is initialied to -1, in case there has been a change in the definition of the boundary conditions between two computations (change in the number or the positions of the walls). Yet, with the $k-\omega$ SST model, the distance to the wall is needed to calculate the turbulent viscosity, which is done before the calculation of the distance to the wall. Hence, when this model is used (and only in that case), ICDPAR is set to 1 by default, to ensure total continuity of the calculation at restart.
As a consequence, with the $k-\omega$ SST model, if the number and positions of the walls are changed at a calculation restart, it is mandatory for the user to set ICDPAR explicitly to -1, otherwise the distance to the wall used will not correspond to the actual position of the walls.
The former algorithm is not compatible with parallelism nor periodicity. Also, whatever the value chosen for ICDPAR, the calculation of the distance to the wall is made

at the most once for all a the beginning of the calculation. It is therefore not compatible with moving walls. Please contact the development team if you need to override this limitation.

The following options are related to ICDPAR=1 or -1. The options of level 2 are described first. Some options are used only in the case of the calculation of the adimensional distance to the wall y^+ (LES model with van Driest damping). Most of these key words are simple copies of the key words for the numerical options of the general equations, with a potentially specific value in the case of the calculation of the distance to the wall.

IWARNY I integer [0] O L2
specifies the level of the output writing concerning the calculation of the distance to the wall with ICDPAR=1 or -1. The higher the value, the more detailled the outputs
useful when ICDPAR=1 or -1

NTCMXY I positive integer [1000] O L2
number of pseudo-time iterations for the calculation of the adimensional distance to the wall y^+
useful when ICDPAR=1 or -1 for the calculation of y^+

NITMAY I integer > 0 [10000] O L3
maximum number of iterations for the solution of the linear systems
useful when ICDPAR=1 or -1

NSWRSY I positive integer [1] O L3
number of iterations for the reconstruction of the right-hand members: corresponds to NSWRSM
useful when ICDPAR=1 or -1

NSWRGY I positive integer [100] O L3
number of iterations for the gradient reconstruction: corresponds to NSWRGR
useful when ICDPAR=1 or -1

IMLIGY I -1, 0 ou 1 [-1 or 1] O L3
type of gradient limitation: corresponds to IMLIGR
useful when ICDPAR=1 or -1

IRCFLY I 0 or 1 [1] O L3
indicates the reconstruction of the convective and diffusive fluxes at the faces: corresponds to IRCFLU
useful when ICDPAR=1 or -1

ISCHCY I 0 or 1 [1] O L3
type of second-order convective scheme: corresponds to ISCHCV
useful when ICDPAR=1 or -1 for the calculation of y^+

ISSTPY I 0 or 1 [0] O L3
indicates if a "slope test" should be used for a second-order convective scheme: corresponds to ISSTPC
useful when ICDPAR=1 or -1 for the calculation of y^+

IMGRPY I 0 or 1 [0] O L3
indicates whether the algebraic multigrid method should be used (IMGR(IVAR)=1) or not (0): corresponds to IMGR
useful when ICDPAR=1 or -1

BLENCY R $0 \leqslant$ real $\leqslant 1$ [0.D0] O L3
proportion of second-order convective scheme: corresponds to BLENCV
useful when ICDPAR=1 or -1 for the calculation of y^+

EPSILY R real number > 0 [1.D-8] O L3
relative precision for the solution of the linear systems: corresponds to EPSILO
useful when ICDPAR=1 or -1

EPSRGY R real number > 0 [1.D-5] O L3
relative precision for the iterative gradient reconstruction: corresponds to EPSRGR
useful when ICDPAR=1 or -1

CLIMGY R real number > 0 [1.5D0] O L3
limitation factor of the gradients: corresponds to CLIMGR
useful when ICDPAR=1 or -1

EXTRAY R 0.D0, 0.5D0 or 1.D0 [0.D0] O L3
extrapolation coefficient of the gradients at the boundaries: corresponds to EXTRAG
useful when ICDPAR=1 or -1

COUMXY R strictly positive real number [5000.D0] O L3
Target Courant number for the calculation of the adimensional distance to the wall
useful when ICDPAR=1 or -1 for the calculation of y^+

EPSCVY R strictly positive real number [1.D-8] O L3
relative precision for the convergence of the pseudo-transient regime for the calculation of the adimensional distance to the wall
useful when ICDPAR=1 or -1 for the calculation of y^+

YPLMXY R real number [200.D0] O L3
value of the adimensional distance to the wall above which the calculation of the distance is not necessary (for the damping)
useful when ICDPAR=1 or -1 for the calculation of y^+

5.2.13 Others

ICCVFG I 0 or 1 [0] O L1
indicates whether the dynamic field should be frozen (1) or not (0)
in such a case, the values of velocity, pressure and the variables related to the potential turbulence model (k, R_{ij}, ε, φ, $\bar{f}$, ω, turbulent viscosity) are kept constant over time and only the equations for the scalars are solved
also, if ICCVFG=1, the physical properties modified in `usphyv` will keep being updated. Beware of non-consistencies if these properties would normally affect the dynamic field (modification of density for instance)
useful if and only if NSCAL > 0 and ISUITE=1

IPUCOU I 0 or 1 [0] O L1
indicates the algorithm for velocity/pressure coupling
= 0: standard algorithm
= 1: reinforced coupling in case calculation with long time steps
always useful (it is seldom advised, but it can prove very useful, for instance, in case of flows with weak convection effects and highly variable viscosity)

ISUIT1 I 0 or 1 [0] O L1
for the 1D wall thermal module, activation (1) or not(0) of the reading of the mesh and of the wall temperature from the FICMT1 restart file
useful if NFPT1D>0.

IMVISF I 0 or 1 [0] O L3
indicates the interpolation method used to project variables from the cell centers to the faces
= 0: linear
= 1: harmonic
always useful

IRCFLU IA 0 or 1 [1] O L2
for each unknown IVAR, IRCFLU(IVAR) indicates whether the convective and diffusive fluxes at the faces should be reconstructed:
= 0: no reconstruction
= 1: reconstruction
deactivating the reconstruction of the fluxes can have a stabilising effect on the calculation. It is sometimes useful with the $k-\varepsilon$ model, if the mesh is strongly non-orthogonal in the near-wall region, where the gradients of k and ε are strong. In such a case, setting IRCFLU(IK(IPHAS))=0 and IRCFLU(IEP(IPHAS))=0 will probably help (switching to a first order convective scheme, BLENCV=0.D0, for k and ε might also help in that case)
always useful

NSWRSM IA positive integer [1, 2, 5 or 10] O L3
for each unknown IVAR, NSWRSM(IVAR) indicates the number of iterations for the reconstruction of the right-hand members of the equations
with a first-order scheme in time (standard case), the default values are 2 for pressure and 1 for the other variables. With a second-order scheme in time (ISCHTP=2) or LES, the default values are 5 for pressure and 10 for the other variables.
useful for all the unknowns

5.3 Numerical, physical and modeling parameters

5.3.1 Numeric Parameters

These parameters correspond to numeric reference values in the code. They can be used but shall not be modified (they are defined as PARAMETER).

ZERO R 0.D0 [O.D0] O L3
Parameter containing the value 0

EPZERO R 1.D-12 [1.D-12] O L3
"Small" real parameter, used for the comparisons of real numbers (absolute value of the difference lower than EPZERO)

PI	R	3.141592653589793D0	[3.141592653589793D0]	O	L3
	Parameter containing the value of π				
GRAND	R	1.D12	[1.D12]	O	L3
	"Large" real parameter, generally used by default as a non physical value for the initialisations of variables which have to be modified by the user				
RINFIN	RR	1.D30	[1.D30]	O	L3
	Real parameter used to represent the "infinite"				

5.3.2 Physical parameters

These parameters correspond to physical reference values in the code. They can be used but shall not be modified (they are defined as PARAMETER).

TKELVI	R	273.15D0	[273.15D0]	O	L3
	Temperature in Kelvin correponding to 0 degrees Celsius.				
TKELVI	R	-273.15D0	[-273.15D0]	O	L3
	Temperature in degrees Celsius corresponding to 0 Kelvin.				
RR	R	8.31434D0	[8.31434D0]	O	L3
	Perfect gas constant in $J/mol/K$				
TREFTH	R	25.D0 + TKELVI	[25.D0 + TKELVI]	O	L3
	Reference temperature for the specific physics, in K				
PREFTH	R	1.01325D5	[1.01325D5]	O	L3
	Reference pressure for the specific physics, in Pa				
VOLMOL	R	22.41D-3	[22.41D-3]	O	L3
	Molar volume under normal pressure and temperature conditions (1 atmosphere, 0°C) in m^{-3}				
STEPHN	R	5.6703D-8	[5.6703D-8]	O	L3
	Stephan constant for the radiative module σ in $W.m^{-2}.K^{-4}$				
PERMVI	R	1.2566D-6	[1.2566D-6]	O	L3
	Vacuum magnetic permeability μ_0 ($=4\pi.10^{-7}$) in $kg.m.A^{-2}.s^{-2}$				
EPSZER	R	8.854D-12	[8.854D-12]	O	L3
	Vacuum permittivity ε_0 in $F.m^{-1}$				

5.3.3 Physical variables

GX,GY,GZ	R	3 real numbers	[0.D0,0.D0,0.D0]	O	L1
	gravity components always useful				

IROVAR IA 0 or 1 [-1] C L1
for each phase IPHAS, IROVAR(IPHAS)=0 indicates that the density is constant. Its value is the reference density RO0(IPHAS).
IROVAR(IPHAS)=1 indicates that the density is variable: its variation law must be given in the user subroutine `usphyv`
negative value: not initialised
always useful

IVIVAR IA 0 or 1 [-1] C L1
for each phase IPHAS, IVIVAR(IPHAS)=0 indicates that the molecular dynamic viscosity is constant. Its value is the reference molecular dynamic viscosity VISCL0(IPHAS).
IVIVAR(IPHAS)=1 indicates that the molecular dynamic viscosity is variable: its variation law must be given in the user subroutine `usphyv`
negative value: not initialised
always useful

RO0 RA real number $\geqslant 0$ [-GRAND*10] C L1
for each phase IPHAS, RO0(IPHAS) is the reference density
negative value: not initialised
its value is not used in gas or coal combustion modeling (it will be calculated following the perfect gas law, with P0 and T0). With the compressible module, it is also not used by the code, but it may be (and often is) referenced by the user in user subroutines; it is therefore better to specify its value.
always useful otherwise, even if a law defining the density is given by the user subroutine `usphyv` or `uselph`
indeed, except with the compressible module, *Code_Saturne* does not use the total pressure P when solving the Navier-Stokes equation, but a reduced pressure
$P^* = P - \rho_0 \underline{g}.(\underline{x} - \underline{x}_0) + P_0^* - P_0$
where $\underline{x}_0$ is a reference point (see XYZP0) and P_0^* and P_0 are reference values (see PRED0 and P0). Hence, the term $-\underline{\text{grad}}\ P + \rho \underline{g}$ in the equation is treated as $-\underline{\text{grad}}\ P^* + (\rho - \rho_0)\underline{g}$. The closer RO0 is to the value of ρ, the more P^* will tend to represent only the dynamic part of the pressure and the faster and more precise its solution will be. Whatever the value of RO0, both P and P^* appear in the listing and the post-processing outputs.
with the compressible module, the calculation is made directly on the total pressure

VISCL0 RA real number > 0 [-GRAND*00] C L1
for each phase IPHAS, VISCL0(IPHAS) is the reference molecular dynamic viscosity
negative value: not initialised
always useful, it is the used value unless the user specifies the viscosity in the subroutine `usphyv`

SRROM R $0 \leqslant$ réel < 1 [-GRAND ou 0] C or O L1
With gas combustion, pulversied coal or the electric module, SRROM is the sub-relaxation coefficient for the density, following the formula:
$\rho^{n+1} = \text{SRROM}\, \rho^n + (1\text{-SRROM})\, \rho^{n+1}$
hence, with a zero value, there is no sub-relaxation. With combustion and pulversied coal, SRROM is initialised to -GRAND and the user must specify a proper value through the Interface or the initialisation subroutines (`usd3p1`, `usebu1`, `uslwc1`, `uscpi1` or `uscpl1`).With the electric module, SRROM is initialised in to 0 and may be modified by the user in `useli1`.
With gas combustion, pulverised coal or electric arc, SSROM is automatically used after the second time-step. With Joule effect, the user decides whether or not it will

be used in `uselph` from the coding law giving the density.

always useful with gas combustion, pulversized coal or the electric module.

P0 RA real number [1.013D5] O L1
for each phase IPHAS, P0(IPHAS) is the reference pressure for the total pressure
except with the compressible module, the total pressure P is evaluated from the reduced pressure P^* so that P is equal to P0 at the reference position $\underline{x}_0$ (given by XYZP0)
with the compressible module, the total pressure is solved directly
always useful

PRED0 RA real number [0.D0] O L3
for each phase IPHAS, PRED0(IPHAS) is the reference value for the reduced pressure P^* (see RO0)
it is especially used to initialise the reduced pressure and as a reference value for the outlet boundary conditions
for an optimised precision in the resolution of P^*, it is wiser to keep PRED0 to 0
with the compressible module, the "pressure" variable appearing in the equations directly represents the total pressure. It is therefore initialised to P0 and not PRED0 (see RO0)
always useful, except with the compressible module

XYZP0 RA 3 real numbers [0.D0,0.D0,0.D0] O L1
for each phase IPHAS, XYZP0(II,IPHAS) is the II coordinate ($1 \leqslant II \leqslant 3$) of the reference point $\underline{x}_0$ for the total pressure
when there are no Dirichlet conditions for the pressure (closed domain), XYZP0 does not need to be specified (unless the total pressure has a clear physical meaning in the configuration treated)
when Dirichlet conditions on the pressure are specified but only through stantard outlet conditions (as it is in most configurations), XYZP0 does not need to be specified by the user, since it will be set to the coordinates of the reference outlet face (*i.e.* the code will automatically select a reference outlet boundary face and set XYZP0 so that P equals P0 at this face). Nontheless, if XYZP0 is pecified by the user, the calculation will remain correct
when direct Dirichlet conditions are specified by the user (specific value set on specific boundary faces), it is better to specify the corresponding reference point (*i.e.* specifiy where the total pressure is P0). This way, the boundary conditions for the reduced pressure will be close to PRED0, ensuring an optimal precision in the resolution. If XYZP0 is not specified, the reduced pressure will be shifted, but the calculations will remain correct.
with the compressible module, the "pressure" variable appearing in the equations directly represents the total pressure. XYZP0 is therefore not used.
always useful, except with the compressible module

T0 RA real number [0.D0] O L1
for each phase IPHAS, T0(IPHAS) is the reference temperature
useful for the specific physics gas or coal combustion (initialisation of the density), for the electricity modules to initialise the domain temperature and for the comperssible module (initialisations). It must be given in Kelvin.

CP0 RA real number > 0 [`-GRAND*10`] O L1
for each phase IPHAS, CP0(IPHAS) is the reference specific heat
useful if there is $1 \leqslant N \leqslant$NSCAUS[42] so that ISCSTH(N)=1 (there is a scalar "temper-

[42] none of the scalars from the specific physics is a temperature

ature"), unless the user specifies the specific heat in the user subroutine `usphyv`[43] (ICP(IPHAS) > 0)
with the compressible module or coal combustion, CP0 is also needed even when there is no user scalar

ICP IA 0 or 1 [0] O L1
for each phase IPHAS, indicates if the specific heat C_p is variable (ICP(IPHAS)=1) or not (0)
When gas or coal combustion is activated, ICP is automatically set to 0 (constant C_p). With the electric module, it is automatically set to 1. The user is not allowed to modify these default choices.
When ICP(IPHAS)=1 is specified, the code automatically modifies this value to make ICP(IPHAS) designate the effective index-number of the property "specific heat of the phase IPHAS". For each cell IEL, the value of C_p is then specified by the user in the appropriate subroutine (`usphyv` for the standard physics) and stored in the array PROPCE(IEL,IPPROC(ICP(IPHAS))) (*see p.59 for specific conditions of use*)
useful if there is 1⩽N⩽NSCAL so that ISCSTH(N)=1 (there is a scalar "temperature") or with the compressible module for non perfect gases

VISLS0 RA real number > 0 [`-GRAND*10`] C L1
VISLS0(J): reference molecular diffusivity related to the scalar J ($kg.m^{-1}.s^{-1}$)
negative value: not initialised
useful if 1⩽J⩽ NSCAL, unless the user specifies the molecular diffusivity in the appropriate user subroutine (`usphyv` for the standard physics) (IVISLS(ISCAL) > 0)
Warning : VISLS0 corresponds to the diffusivity. For the temperature, it is therefore defined as λ/C_p where λ and C_p are the conductivity and specific heat. When using the Graphical Inteface, λ and C_p are specified separately, and VISLS0 is calculated automatically
With the compressible module, VISLS0 (given in `uscfxi2`) is directly the thermal conductivity $W.m^{-1}.K^{-1}$
With gas or coal combustion, the molecular diffusivity of the enthalpy ($kg.m^{-1}.s^{-1}$) must be specified by the user in the variable DIFTL0 (`usebu1`, `usd3p1`, `uslwc1`, `uscpi1`, `uscpl1`)
With the electric module, for the Joule effect, the diffusivity is specified by the user in `uselph` (even if it is constant). For the electric arc, it is calculated from the thermochemical data file

IVISLS IA positive or zero integer [0] O L1
indicates if the viscosity related to the scalar ISCAL is variable (IVISLS(ISCAL)=1) or not (0). The user must specify IVISLS only for the user scalars (ISCAL ⩽ NSCAUS).
When IVISLS(ISCAL)=1 is specified, the code automatically modifies this value to make IVISLS(ISCAL) designate the effective index-number of the property "diffusivity of the scalar ISCAL". For each cell IEL, the value is then specified by the user in the appropriate subroutine (`usphyv` for the standard physics) and stored in the array PROPCE(IEL,IPPROC(IVISLS(IPHAS))) (*see p.59 for specific conditions of use*)
useful if 1⩽N⩽NSCAL

DIFTL0 R real number > 0 [`-GRAND`] C L1
molecular diffusivity for the enthalpy ($kg.m^{-1}.s^{-1}$) for gas or coal combustion (the code then automatically sets VISLS0 to DIFTL0 for the scalar representing the enthalpy)
always useflu for gas or coal combustion

[43] when using the Graphical Interface, CP0 is also used to calculate the diffusivity of the thermal scalars, based on their conductivity; it is therefore needed, unless the diffusivity is also specified in `usphyv`

SCAMIN RA real number [GRAND] O L1
SCAMIN(ISCAL) is the lower limit value for the scalar ISCAL. At each time step, in every cell where the calculated value for RTP(IEL,ISCA(ISCAL)) is lower than SCAMIN(ISCAL), RTP(IEL,ISCA(ISCAL)) will be reset to SCAMIN(ISCAL)
there is no limitation if SCAMIN(ISCAL)>SCAMAX(ISCAL)
SCAMIN shall not be specified for non-user scalars (specific physics) or for scalar variances
useful if and only if 1⩽ISCAL⩽ NSCAUS

SCAMAX RA real number [-GRAND] O L1
SCAMAX(ISCAL) is the higher limit value for the scalar ISCAL. At each time step, in every cell where the calculated value for RTP(IEL,ISCA(ISCAL)) is higher than SCAMAX(ISCAL), RTP(IEL,ISCA(ISCAL)) will be reset to SCAMAX(ISCAL)
there is no limitation if SCAMIN(ISCAL)>SCAMAX(ISCAL)
SCAMAX shall not be specified for non-user scalars (specific physics) or for scalar variances
useful if and only if 1⩽ISCAL⩽ NSCAUS

SIGMAS RA real number > 0 [1D0] O L2
SIGMAS(ISCAL): turbulent Prandtl (or Schmidt) number for the scalar ISCAL
useful if and only if 1⩽ISCAL⩽ NSCAUS

RVARFL RA real number > 0 [0.8D0] O L2
when ISCAVR(ISCAL)>0, RVARFL(ISCAL) is the coefficient R_f in the dissipation term $-\frac{\rho}{R_f}\frac{\varepsilon}{k}$ of the equation concerning the scalar ISCAL, which represents the root mean square of the fluctuations of the scalar ISCAVR(ISCAL)
useful if and only if there is 1⩽ISCAL⩽ NSCAL such as ISCAVR(ISCAL)>0

5.3.4 Modeling parameters

XLOMLG RA real number > 0 [-GRAND*10] O L1
for each phase IPHAS, XLOMLG(IPHAS) is the mixing length
useful if and only if there is a phase IPHAS so that ITURB(IPHAS)= 10 (mixing length)

ALMAX RA -GRAND, real number > 0 [-GRAND*10] O L2
for each phase IPHAS, ALMAX(IPHAS) is a characteristic macroscopic length of the domain, used for the initialisation of the turbulence and the potential clipping (with ICLKEP(IPHAS)=1)
negative value: not initialised (the code then uses the cubic root of the domain volume)
useful if and only if there is a phase IPHAS such as TURB(IPHAS)= 20, 21, 30, 31, 50 or 60 (RANS models)

UREF RA real number > 0 [-GRAND*10] C L1
for each phase IPHAS, UREF(IPHAS) is the characteristic flow velocity, used for the initialisation of the turbulence
negative value: not initialised
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)= 20, 21, 30, 31, 50 ou 60 (RANS model) and the turbulence is not initialised somewhere else (restart file or subroutine `usiniv`)

Basic constants of the $k-\varepsilon$ and the other RANS models

XKAPPA R real number > 0 [0.42D0] O L3
Kármán constant
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)$\geqslant$10 (mixing length, $k-\varepsilon$, $R_{ij}-\varepsilon$, LES, v2f or $k-\omega$)

CSTLOG R real number > 0 [5.2D0] O L3
constant of the logarithmic wall function
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)$\geqslant$10 (mixing length, $k-\varepsilon$, $R_{ij}-\varepsilon$, LES, v2f or $k-\omega$)

CMU R real number > 0 [0.09D0] O L3
constant C_μ for all the RANS turbulence models except for the v2f model (see CV2FMU for the value of C_μ in case of v2f modeling)
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)= 20, 21, 30, 31 or 60 ($k-\varepsilon$, $R_{ij}-\varepsilon$ or $k-\omega$)

CE1 R real number > 0 [1.44D0] O L3
constant $C_{\varepsilon 1}$ for all the RANS turbulence models except for the v2f and the $k-\omega$ models
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)= 20, 21, 30 or 31 ($k-\varepsilon$ or $R_{ij}-\varepsilon$)

CE2 R real number > 0 [1.92D0] O L3
constant $C_{\varepsilon 2}$ for the $k-\varepsilon$ and $R_{ij}-\varepsilon$ LRR models
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)= 20, 21 or 30 ($k-\varepsilon$ or $R_{ij}-\varepsilon$ LRR)

CE4 R real number > 0 [1.2D0] O L3
constant $C_{\varepsilon 4}$ for the interfacial term (Lagrangian module) in case of two-way coupling
useful in case of Lagrangian modeling, in $k-\varepsilon$ and $R_{ij}-\varepsilon$ with two-way coupling

SIGMAK R real number > 0 [1.00D0] O L3
Prandtl number for k with $k-\varepsilon$ and v2f models
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=20, 21 or 50 ($k-\varepsilon$ or v2f)

SIGMAE R real number > 0 [1.30D0] O L3
Prandtl number for ε
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)= 20, 21, 30, 31 or 50 ($k-\varepsilon$, $R_{ij}-\varepsilon$ or v2f)

Constants specific to the $R_{ij}-\varepsilon$ LRR model (ITURB=30)

CRIJ1 R real number > 0 [1.8D0] O L3
constant C_1 for the $R_{ij}-\varepsilon$ LRR model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=30 ($R_{ij}-\varepsilon$ LRR)

CRIJ2 R real number > 0 [0.6D0] O L3
constant C_2 for the $R_{ij} - \varepsilon$ LRR model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=30 ($R_{ij} - \varepsilon$ LRR)

CRIJ3 R real number > 0 [0.55D0] O L3
constant C_3 for the $R_{ij} - \varepsilon$ LRR model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=30 ($R_{ij} - \varepsilon$ LRR)

CRIJEP R real number > 0 [0.18D0] O L3
constant C_ε for the $R_{ij} - \varepsilon$ LRR model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=30 ($R_{ij} - \varepsilon$ LRR)

CSRIJ R real number > 0 [0.22D0] O L3
constant C_s for the $R_{ij} - \varepsilon$ LRR model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=30 ($R_{ij} - \varepsilon$ LRR)

CRIJP1 R real number > 0 [0.5D0] O L3
constant C_1' for the $R_{ij} - \varepsilon$ LRR model, corresponding to the wall echo terms
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=30 and IRIJEC(IPHAS)=1 ($R_{ij} - \varepsilon$ LRR)

CRIJP2 R real number > 0 [0.3D0] O L3
constant C_2' for the $R_{ij} - \varepsilon$ LRR model, corresponding to the wall echo terms
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=30 and IRIJEC(IPHAS)=1 ($R_{ij} - \varepsilon$ LRR)

Constants specific to the $R_{ij} - \varepsilon$ SSG model

CSSGS1 R real number > 0 [1.7D0] O L3
constant C_{s1} for the $R_{ij} - \varepsilon$ SSG model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=31 ($R_{ij} - \varepsilon$ SSG)

CSSGS2 R real number > 0 [-1.05D0] O L3
constant C_{s2} for the $R_{ij} - \varepsilon$ SSG model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=31 ($R_{ij} - \varepsilon$ SSG)

CSSGR1 R real number > 0 [0.9D0] O L3
constant C_{r1} for the $R_{ij} - \varepsilon$ SSG model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=31 ($R_{ij} - \varepsilon$ SSG)

CSSGR2 R real number > 0 [0.8D0] O L3
constant C_{r2} for the $R_{ij} - \varepsilon$ SSG model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=31 ($R_{ij} - \varepsilon$ SSG)

CSSGR3 R real number > 0 [0.65D0] O L3
constant C_{r3} for the $R_{ij} - \varepsilon$ SSG model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=31 ($R_{ij} - \varepsilon$ SSG)

CSSGR4 R real number > 0 [0.625D0] O L3
constant C_{r4} for the $R_{ij} - \varepsilon$ SSG model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=31 ($R_{ij} - \varepsilon$ SSG)

CSSGR5 R real number > 0 [0.2D0] O L3
constant C_{r1} for the $R_{ij} - \varepsilon$ SSG model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=31 ($R_{ij} - \varepsilon$ SSG)

CSSGE2 R real number > 0 [1.83D0] O L3
constant $C_{\varepsilon 2}$ for the $R_{ij} - \varepsilon$ SSG model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=31 ($R_{ij} - \varepsilon$ SSG)

Constants specific to the v2f φ-model

CV2FA1 R real number > 0 [0.05D0] O L3
constant a_1 for the v2f φ-model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=50 (v2f φ-model)

CV2FE2 R real number > 0 [1.85D0] O L3
constant $C_{\varepsilon 2}$ for the v2f φ-model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=50 (v2f φ-model)

CV2FMU R real number > 0 [0.22D0] O L3
constant C_μ for the v2f φ-model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=50 (v2f φ-model)

CV2FC1 R real number > 0 [1.4D0] O L3
constant C_1 for the v2f φ-model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=50 (v2f φ-model)

CV2FC2 R real number > 0 [0.3D0] O L3
constant C_2 for the v2f φ-model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=50 (v2f φ-model)

CV2FCT R real number > 0 [6.D0] O L3
constant C_T for the v2f φ-model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=50 (v2f φ-model)

CV2FCL R real number > 0 [0.25D0] O L3
constant C_L for the v2f φ-model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=50 (v2f φ-model)

CV2FET R real number > 0 [110.D0] O L3
constant C_η for the v2f φ-model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=50 (v2f φ-model)

Constants specific to the $k - \omega$ SST model

CKWSK1 R real number > 0 [1.D0/0.85D0] O L3
constant σ_{k1} for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)

CKWSK2 R real number > 0 [2.D0] O L3
constant σ_{k2} for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)

CKWSW1 R real number > 0 [2.D0] O L3
constant $\sigma_{\omega 1}$ for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)

CKWSW2 R real number > 0 [1.D0/0.856D0] O L3
constant $\sigma_{\omega 2}$ for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)

CKWBT1 R real number > 0 [0.075D0] O L3
constant β_1 for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)

CKWBT2 R real number > 0 [0.0828D0] O L3
constant β_2 for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)

CKWGM1 R real number > 0 $[\frac{\beta_1}{C_\mu} - \frac{\kappa^2}{\sqrt{C_\mu}\sigma_{\omega 1}}]$ O L3
constant γ_1 for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)
Warning: γ_1 is calculated before the call to **`usini1`**. *Hence, if β_1, C_μ, κ or $\sigma_{\omega 1}$ is modified in* **`usini1`**, *CKWGM1 must also be modified in accordance*

CKWGM2 R real number > 0 $[\frac{\beta_2}{C_\mu} - \frac{\kappa^2}{\sqrt{C_\mu}\sigma_{\omega 2}}]$ O L3
constant γ_2 for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)
Warning: γ_2 is calculated before the call to **`usini1`**. *Hence, if β_2, C_μ, κ or $\sigma_{\omega 2}$ is modified in* **`usini1`**, *CKWGM2 must also be modified in accordance*

CKWA1 R real number > 0 [0.31D0] O L3
constant a_1 for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)

CKWC1 R real number > 0 [10.D0] O L3
constant c_1 for the $k-\omega$ SST model
useful if and only if there is a phase IPHAS such as ITURB(IPHAS)=60 ($k-\omega$ SST)

5.4 Thermal radiative transfers: global settings

All the following key words may be modified in the user subroutines `usray*` (or, for some of them, by through the thermochemical data files). It is however not recommended to modify those which do not belong to level L1.

IRAYON IA 0, 1, 2 [0] O L1
for each phase IPHAS, IRAYON(IPHAS) activates (> 0) or deactivates (=0) the radiation module
if a specific physics is activated (in that case, NSCAPP>0), IRAYON(IPHAS) must be kept to 0 (see IRAYPP)
The different values correspond to the following modelings:
= 1 discrete ordinates (standard option for radiation in semi-transparent media)
= 2 "P-1" model
Warning: the P-1 model allows faster computations, but it may only be applied to media with uniform large optical thickness, such as some cases of pulverised coal combustion

IRAYPP I 0, 1, 2, 3 or 4 [0] O L1
when a specific physics is activated[44] (NPHAS=1, compulsory) IRAYPP indicates if thermal radiative transfers are calculated (> 0) or not (=0).
The value of IRAYPP is given *via* a data file (gas combustion: *dp_C3P*, *dp_C3PSJ*, or *dp_C4P*; pulverised coal combustion: *dp_FCP*; electric module: *dp_ELE*)
IRAYPP allows to choose between the discrete ordinates method and the P-1 method (see IRAYON) and to choose the method used to calculate the absorption coefficient. The absorption coefficient may be set by the user in the data file (then, IMODAK=0) or calculated using "Modak[45]" (then, IMODAK=1). The options are the followings:
= 1 discrete ordinates method with the absorption coefficient given by the user in the data file (IMODAK=0)
= 2 discrete ordinates method using Modak for the calculation of the absorption coefficient (IMODAK=1)
= 3 "P-1" model with the absorption coefficient given by the user in the data file (IMODAK=0)
= 4 "P-1" model using Modak for the calculation of the absorption coefficient (IMODAK=1)
For the electric module, IRAYPP is not set directly in the data file, but deduced from the type of XKABEL specified in the file (given by IXKABE). In that case, IRAYPP can only be equal to 0 (IXKABE=0 or 2) or 1 (IXKABE=1)

IMODAK I 0 or 1 [0] O L3
when gas or coal combustion is activated, IMODAK indicates whether the absorption coefficient shall be calculated "automatically" (=1) or read from the data file (=0) (see IRAYPP)
useful if the radiation module is activated; IMODAK is then automatically set from the value of IRAYPP, without intervention of the user

ISUIRD I 0 or 1 [ISUITE] C L1
indicates whether the radiation variables should be initialised (=0) or read from a restart file (=1)
useful if and only if the radiation module is activated (in this case, a restart file *rayamo* must be available)

NFREQR I strictly positive integer [1] O L1
period of the radiation module
the radiation module is called every NFREQR time steps (more precisely, every time NTCABS is a multiple of NFREQR). Also, in order to have proper initialisation of

[44] except with the compressible module, which is not compatible with radiation
[45] for details about the calculation of the absorption coefficient, please refer to MODAK A.T., "Radiation from products of combustion"

the variables, whatever the value of NFREQR, the radiation module is called at the first time step of a calculation (restart or not)
useful if and only if the radiation module is activated

NDIREC I 32 ou 128 [32] O L1
number of directions for the angular discretisation of the radiation propagation with the DOM model (IRAYON=1)
no other possible value, because of the way the directions are calculated
the calculation with 32 directions may break the symmetry of physically axisymmetric cases (but the cost in CPU time is much lower than with 128 directions)
useful if and only if the radiation module is activated with the DOM method

XNP1MX R real number [10] O L3
with the P-1 model (IRAYON=2), XNP1MX is the percentage of cells of the calculation domain for which it is acceptable that the optical thickness is lower than unity[46], although it is not to be desired
useful if and only if the radiation module is activated with the P-1 method

IDIVER I 0, 1 or 2 [2] C L1
indicates the method used to calculate the radiative source term:
= 0: semi-analytic calculation (compulsory with transparent media)
= 1: conservative calculation
= 2: semi-analytic calculation corrected in order to be globally consevative
useful if and only if the radiation module is activated
Note: if the medium is transparent, the choice has no effect on the calculation

IIMPAR I 0, 1 or 2 [1] O L1
choice of the display level in the listing concerning the calculation of the wall temperatures:
= 0: no display
= 1: standard
= 2: complete
useful if and only if the radiation module is activated

IIMLUM I 0, 1 or 2 [1] O L1
choice of the display level in the listing concerning the solution of the radiative transfer equation:
= 0: no display
= 1: standard
= 2: complete
useful if and only if the radiation module is activated

NBRVAP CA string of less than 80 characters [name_IPHAS] O L1
name associated for the post-processing to each of the following variables, defined at the cell centers (*see* [5] for more details concerning their definitions):
NBRVAP(ITSRAY,IPHAS): radiative source term (W/m^3)
NBRVAP(IQRAYP,IPHAS): radiative flux density vector (W/m^2)
NBRVAP(IABSP,IPHAS): absorption part in the source term (W/m^3)
NBRVAP(IEMIP,IPHAS): emission part in the source term (W/m^3)
NBRVAP(ICAKP,IPHAS): absorption coefficient of the medium (m^{-1})

[46] more precisely, where KL is lower than 1, where K is the absorption coefficient of the medium and L is a characteristic length of the domain

the default values are:
NBRVAP(ITSRAY,IPHAS) = Srad_IPHAS
NBRVAP(IQRAYP,IPHAS) = Qrad_IPHAS
NBRVAP(IABSP,IPHAS) = Absorp_IPHAS
NBRVAP(IEMIP,IPHAS) = Emiss_IPHAS
NBRVAP(ICAKP,IPHAS) = CoefAb_IPHAS
useful if and only if the radiation module is activated

IRAYVP IA -1 or 1 [-1] O L1
activates (=1) or deactivates (=-1) the post-processing for the each of the followiing variables defined at the cell centers:
IRAYVP(ITSRAY,IPHAS): radiative source term (W/m^3)
IRAYVP(IQRAYP,IPHAS): radiative flux density vector (W/m^2)
IRAYVP(IABSP,IPHAS): absorption part in the source term (W/m^3)
IRAYVP(IEMIP,IPHAS): emission part in the source term (W/m^3)
IRAYVP(ICAKP,IPHAS): absorption coefficient of the medium (m^{-1})
useful if and only if the radiation module is activated

NBRVAF CA string of less than 80 characters [name_IPHAS] O L1
name associated for the post-processing to each of the following variables, defined at the boundary faces (*see* [5] for more details concerning their definitions):
NBRVAF(ITPARP,IPHAS): wall temperature at the boundary faces (K)
NBRVAF(IQINCP,IPHAS): radiative incident flux density (W/m^2)
NBRVAF(IXLAMP,IPHAS): thermal conductivity of the boundary faces ($W/m/K$)
NBRVAF(IEPAP,IPHAS): wall thickness (m)
NBRVAF(IEPSP,IPHAS): wall emissivity
NBRVAF(IFNETP,IPHAS): net radiative flux density (W/m^2)
NBRVAF(IFCONP,IPHAS): convective flux density (W/m^2)
NBRVAF(IHCONP,IPHAS): convective exchange coefficient ($W/m^2/K$)
The default values are:
NBRVAF(ITPARP,IPHAS) = Temp_paroi_IPHAS
NBRVAF(IQINCP,IPHAS) = Flux_incident_IPHAS
NBRVAF(IXLAMP,IPHAS) = Conductivite_th_IPHAS
NBRVAF(IEPAP,IPHAS) = Epaisseur_IPHAS
NBRVAF(IEPSP,IPHAS) = Emissivite_IPHAS
NBRVAF(IFNETP,IPHAS) = Flux_net_IPHAS
NBRVAF(IFCONP,IPHAS) = Flux_convectif_IPHAS
NBRVAF(IHCONP,IPHAS) = Coef_ech_convectif_IPHAS
useful if and only if the radiation module is activated

IRAYVF IA -1 or 1 [-1] O L1
activates (=1) or deactivates (=-1) the post-processing for each of the followiing variables defined at the boundary faces:
IRAYVF(ITPARP,IPHAS): wall temperature at the boundary faces (K)
IRAYVF(IQINCP,IPHAS): radiative incident flux density (W/m^2)
IRAYVF(IXLAMP,IPHAS): thermal conductivity of the boundary faces ($W/m/K$)
IRAYVF(IEPAP,IPHAS): wall thickness (m)
IRAYVF(IEPSP,IPHAS): wall emissivity
IRAYVF(IFNETP,IPHAS): net radiative flux density (W/m^2)
IRAYVF(IFCONP,IPHAS): convective flux density (W/m^2)
IRAYVF(IHCONP,IPHAS): convective exchange coefficient ($W/m^2/K$)
useful if and only if the radiation module is activated

TMIN R real number positif [0.D0] O L3
minimum allowed value for the wall temperatures in Kelvin
useful if and only if the radiation module is activated

TMAX R real number positif [GRAND + 273.15D0] O L3
maximum allowed value for the wall temperatures in Kelvin
useful if and only if the radiation module is activated

5.5 Electric module (Joule effect and electric arc): specificities

The electric module is composed of a Joule effect module (IPPMOD(IELJOU)) and an electric arc module (IPPMOD(IELARC)).

The Joule effect module is designed to take into account the Joule effect (for instance in glass furnaces) with real or complex potential in the enthalpy equation. The Laplace forces are not taken into account in the impluse momentum equation. Specific boundary conditions can be applied to account for the coupled effect of transformers (offset) in glass furnaces.

The electric arc module is designed to take into account the Joule effect (only with real potential) in the enthalpy equation. The Laplace forces are taken into account in the impulse momentum equation.

The key words used in the global settings are quite few. They are found in the subroutine `useli1` (see the description of this user subroutine §4.37).

IELCOR I 0, 1 [0] O L1
when IELCOR=1, the boundary conditions for the potential will be tuned at each time step in order to reach a user-specified target dissipated power PUISIM (Joule effect) or a user-specified target current intensity COUIMP (electric arc)
the boundary condition tuning is controlled by the subroutine `uselrc`
alway useful

COUIMP R real number $\geqslant 0$ [0] O L1
with the electric arc module, COUIMP is the target current intensity (A) for the calculations with boundary condition tuning for the potential
the target intensity will be reached if the boundary conditions are expressed using the variable DPOT or if the initial boundary conditions are multiplied by the variable COEJOU
useful with the electric arc module if IELCOR=1

PUISIM R real number $\geqslant 0$ [0] O L1
with the Joule effect module, PUISIM is the target dissipated power (W) for the calculations with boundary condition tuning for the potential
the target power will be reached if the boundary conditions are expressed using the variable DPOT or if the initial boundary conditions are multiplied by the variable COEJOU
useful with the Joule effect module if IELCOR=1

DPOT R real number $\geqslant 0$ [0] O L1
DPOT is the potential difference (V) which generates the current (and the Joule effect) for the calculations with boundary conditions tuning for the potential. This value is initialised set by the user (`useli1`). It is then automatically tuned depending on the value of dissipated power (Joule effect module) or the intensity of current (electric arc module). In order for the correct power or intensity to be reached, the boundary conditions for the potential must be expressed with DPOT (`uselcl`). The tuning can

be controlled in `uselrc`
useful if IELCOR=1

COEJOU R real number $\geqslant 0$ [1] O L2
only with the Joule effect, COEJOU can be used if the user does not wish to use DPOT. COEJOU is the coefficient to be applied to the initial potential difference to reach the target dissipated power. Its value is automatically initialised to 1 and is updated during the calculation. In order for the correct power to be reached, the boundary conditions for the potential must be expressed with COEJOU (`uselcl`). The tuning can be controlled in `uselrc`
Useful if IELCOR=1

5.6 Compressible module: specificities

The key words used in the global settings are quite few. They are found in the subroutines `uscfx1` and `uscfx2` (see the description of these user subroutines, §4.40.1).

ICFGRP IA 0 or 1 [1] C L1
for each phase IPHAS, ICFGRP(IPHAS) indicates if the boundary conditions should take into account (=1) or not (=0) the hydrostatic balance.
always useful.
In the cases where gravity is predominant, taking into account the hydrostatic pressure allows to get rid of the disturbances which may appear near the horizontal walls when the flow is little convective.
Otherwise, when ICFGRP=0, the pressure condition is calculated from the solution of the unidimensional Euler equations for a perfect gas near a wall, for the variables "normal velocity", "density" and "pressure":

Case of an expansion ($M \leqslant 0$):

$$\begin{cases} P_p = 0 & \text{if} \quad 1 + \dfrac{\gamma-1}{2} M < 0 \\ P_p = P_i \left(1 + \dfrac{\gamma-1}{2} M\right)^{\frac{2\gamma}{\gamma-1}} & \text{otherwise} \end{cases}$$

Case of a shock ($M > 0$):

$$P_p = P_i \left(1 + \frac{\gamma(\gamma+1)}{4} M^2 + \gamma M \sqrt{1 + \frac{(\gamma+1)^2}{16} M^2}\right)$$

with $M = \dfrac{\underline{u_i} \cdot \underline{n}}{c_i}$, internal Mach number calculated with the variables taken in the cell adjacent to the wall.

IVISCV IA 0 or 1 [0] C L1
for each phase IPHAS, IVISCV(IPHAS)=0 indicates that the volume viscosity is constant and equal to the reference volume viscosity VISCV0(IPHAS).
IVISCV(IPHAS)=1 indicates that the volume viscosity is variable: its variation law must be specified in the user subroutine `uscfpv`.
always useful
The volume viscosity κ is defined by the formula expressing the stress:

$$\underline{\underline{\sigma}} = -P\,\underline{\underline{Id}} + \mu(\underline{\text{grad}}\ \underline{u} + {}^t\underline{\underline{\text{grad}}}\ \underline{u}) + (\kappa - \frac{2}{3}\mu)\,\text{div}(\underline{u})\,\underline{\underline{Id}} \qquad (4)$$

VISCV0 RA real number ≥ 0 [0.D0] O L1
for each phase IPHAS, VISCV0(IPHAS) is the reference volume viscosity (noted κ in the equation expressing $\underline{\underline{\sigma}}$ in the paragraph dedicated to IVISCV)
always useful, it is the used value, unless the user specifies the volume viscosity in the user subroutine `uscfpv`

IGRDPP I 0 ou 1 [0] O L3
indicates whether the pressure should be updated (=1) or not (=0) after the solution of the acoustic equation
always useful

5.7 Lagrangian multiphase flows

Most of these key words may be modified in the user subroutines `uslag1`, `uslag2`, `uslabo`, `uslaen`, `uslast` and `uslaed`. It is however strongly recommended not to modify those belonging to the level L3.

First of all, it should be noted that the Lagrangian module is compliant with all the RANS turbulence models and with laminar flows. However, the particule turbulent diffusion is not specially adapted to the second order $R_{ij} - \varepsilon$ models. The same isotropic model is used as in the $k - \varepsilon$ models, with k calculated from the trace of R_{ij}. Also, two-way coupling is not compatible with the $k - \omega$ SST model.

5.7.1 Global settings

IILAGR I 0, 1, 2, 3 [0] C L1
activates (>0) or deactivates (=0) the Lagrangian module
the different values correspond to the following modelings:
= 1 Lagrangian two-phase flow in one-way coupling (no influence of the particles on the continuous phase)
= 2 Lagrangian two-phase flow with two-way coupling (influence of the particles on the dynamics of the continuous phase). It must be noted that the two-way coupling is taken into account only for the first eulerian phase. Dynamics, temperature and mass may be coupled independently
= 3 Lagrangian two-phase flow on frozen continuous phase. This option can only be used in case of a calculation restart (ISUITE = 1). All the eulerian fields are frozen (including the scalar fields). This option automatically implies ICCVFG = 1
always useful

ISUILA I 0, 1 [0] C L1
activation (=1) or not (=0) of a Lagrangian calculation restart. The calculation restart file read when this option is activated (FICAML) only contains the data related to the particles (see also ISUIST)
the global calculation must also be a restart calculation (ISUITE=1)
always useful

ISUIST I 0, 1 [0] C L1
during a Lagrangian calculation restart, indicates whether the particle statistics (volume and boundary) and two-way coupling terms are to be read from a restart file (=1) or reinitialised (=0). The file to be read is FICMLS
useful if ISUILA = 1

NBPMAX I positive or null integer [1000] C L1
maximum number of particles allowed simultaneously in the calculation domain. It must be reminded that the required memory evolves accordingly

NBPART I positive or null integer [0] O L3
number of particles treated during one Lagrangian time step
NBPART must always be lower than NBPMAX
always useful, but initialised and updated without intervention of the user

NVLS I integer between 0 and 10 [0] O L2
number of additional variables related to the particles
the additional variables can be accessed in the arrays ETTP and ETTPA by means of the pointer JVLS: ETTP(NBPT,JVLS(II)) and ETTPA(NBPT,JVLS(II)) (NBPT is the index-number of the treated particle, and II an integer between 1 and NVLS)

ISTTIO I 0, 1 [0] C L1
indicates the steady (=1) or unsteady (=0) state of the continuous phase flow
in particular, ISTTIO = 1 is needed in order to:
calculate stationary statistics in the volume or at the boundaries (starting respectively from the Lagrangian iterations NSTIST and NSTBOR)
calculate time-averaged two-way coupling source terms (from the Lagrangian iteration NSTITS)
useful if IILAGR=1 or IILAGR=2 (if IILAGR=3, then ISTTIO=1 automatically)

INJCON I 0, 1 [0] O L1
activates (=1) or not (=0) the continuous injection of particles
this option allows to inject particles continuously during the duration of the Lagrangian time step DTP rather than only once at the beginning of the Lagrangian iteration. It helps avoiding the fractioning of the particle cloud close to the injection areas

IROULE I 0, 1 [0] O L1
activates (=1) or not (=0) of the particle cloning/fusion technique (option also called "Russian roulette")
when IROULE = 1, the importance function must be specified *via* the array CROULE in the user subroutine `uslaru`

ISUIVI I 0, 1 [0 or 1] O L2
specifies if a particle should be followed (=1) or will disappear from the domain (=0) after an interaction with a boundary:
= 0: the particle must not be followed in the calculation domain after an iteraction between its trajectory and a boundary face, for instance entry (IENTRL), outlet (ISORTL), definitive deposition on a wall (IDEPO1, IDEPO2)
= 1: the particle must still be followed in the calculation domain after an iteraction between its trajectory and a boundary face, for instance rebound (IREBOL), deposition with potential resuspension (IDEPO3)
the value of ISUIVI (ISUIVI = 0 or ISUIVI = 1) for a type of interaction can be defined as a function of the particle behaviour or properties. It is for example the default case for the fouling interaction type (IENCRL)
always useful

TTCLAG R positive real number [0] O L3
physical time of the Lagrangian simulation
always useful

IPLAS I integer > 0 [1] O L3
absolute iteration number (including the restarts) in the Lagrangian module (*i.e.* Lagrangian time step number)
always useful

5.7.2 Specific physics models associated with the particles

IPHYLA I 0, 1, 2 [0] C L1
activates (>0) or deactivates (=0) the physical models associated to the particles:
= 1: allows to associate with the particles evolution equations on their temperature (in degrees Celsius), their diameter and their mass
= 2: the particles are pulverised coal particles. Evolution equations on temperature (in degree Celsius), mass of reactive coal, mass of char and diameter of the shrinking core are associated with the particles. This option is available only if the continuous phase represents a pulverised coal flame
always useful

IDPVAR I 0, 1 [0] O L1
activation (=1) or not (=0) of an evolution equation on the particle diameter
useful if IPHYLA = 1

ITPVAR I 0, 1 [0] O L1
activation (=1) or not (=0) of an evolution equation on the particle temperature (in degrees Celsius)
useful if IPHYLA = 1 and if there is a thermal scalar associated with the continuous phase

IMPVAR I 0, 1 [0] O L1
activation (=1) or not (=0) of an evolution equation on the particle mass
useful if si IPHYLA = 1

TPART R real number > TKELVN [700.D0] O L1
initialisation temperature (in degree Celsius) for the particles already present in the calculation domain when an evolution equation on the particle temperature is activated during a calculation (IPHYLA = 1 and ITPVAR = 1)
useful if ISUILA = 1 and ITPVAR = 0 in the previous calculation

CPPART R positive real number [5200.D0] O L1
initialisation value for the specific heat ($J.kg^{-1}.K^{-1}$) of the particles already present in the calculation domain when an evolution equation on the particle temperature is activated during a calculation (IPHYLA = 1 and ITPVAR = 1)
useful if ISUILA = 1 and ITPVAR = 0 in the previous calculation

IENCRA I 0, 1 [0] O L1
activates (=1) or not (=0) the option of coal particle fouling. It then is necessary to specify the domain boundaries on which fouling may take place.
useful if IPHYLA = 2

TPRENC R real number > TKELVN [600.D0] O L1
limit temperature (in degree Celsius) below which the coal particles do not cause any

fouling (if the fouling model is activated)
useful if IPHYLA = 2 and IENCRA = 1

VISREF R positive real number [10000.D0] O L1
ash critical viscosity in $kg.m^{-1}.s^{-1}$, in the fouling model [47]
useful if IPHYLA = 2 and IENCRA = 1

5.7.3 Options for two-way coupling

NSTITS I strictly positive integer [1] O L1
number of absolute Lagrangian iterations (including the restarts) after which a time-average of the two-way coupling source terms is calculated
indeed, if the flow is steady (ISTTIO=1), the average quantities that appear in the two-way coupling source terms can be calculated over different time steps, in order to get a better precision
if the number of absolute Lagrangian iterations is strictly inferior to NSTITS, the code considers that the flow has not yet reached its steady state (transition period) and the averages appearing in the source terms are reinitialised at each time step, as it is the case for unsteady flows (ISTTIO=0)
useful if IILAGR = 2 and ISTTIO = 1

LTSDYN I 0, 1 [0] O L1
activation (=1) or not (=0) of the two-way coupling on the dynamics of the continuous phase
useful if IILAGR = 2 and ICCVFG = 0

LTSMAS I 0, 1 [0] O L1
activation (=1) or not (=0) of the two-way coupling on the mass
useful if IILAGR = 2, IPHYLA = 1 and IMPVAR = 1

LTSTHE I 0, 1 [0] O L1
if IPHYLA = 1 and ITPVAR = 1, LTSTHE activates (=1) or not (=0) the two-way coupling on temperature
if IPHYLA = 2, LTSTHE activates (=1) or not (=0) the two-way coupling on the eulerian variables related to pulverised coal combustion
useful if IILAGR = 2

5.7.4 Numerical modeling

NORDRE I 1, 2 [2] O L2
order of integration for the stochastic differential equations
= 1 integration using a first-order scheme
= 2 integration using a second-order scheme
always useful

ILAPOI I 0, 1 [0] O L3
activation (=1) or not (=0) of the solution of a Poisson's equation for the correction of the particle instantaneous velocities (in order to obtain a null divergence)

[47] J.D. Watt et T. Fereday (*J.Inst.Fuel*, Vol.42-p99)

this option is not validated and reserved to the development team. Do not change the default value

IDISTU I 0, 1 [1] O L3
activation (=1) or not (=0) of the particle turbulent dispersion
the turbulent dispersion is compatible only with the RANS turbulent models ($k-\varepsilon$, $R_{ij}-\varepsilon$, v2f or $k-\omega$)
(ITURB(IPHAS)=20, 21, 30, 31, 50 or 60 with IPHAS = 1)
always useful

IDIFFL I 0, 1 [0] O L3
IDIFFL=1 suppresses the crossing trajectory effect, making turbulent dispersion for the particles identical to the turbulent diffusion of fluid particles
useful if IDISTU=1

MODCPL I positive integer [0] O L1
activates (>0) or not (=0) the complete turbulent dispersion model
when MODCPL is strictly positive, its value is interpreted as the absolute Lagrangian time step number (including restarts) after which the complete model is applied
since the complete model uses volume statistics, MODCPL must either be 0 or be larger than IDSTNT
useful if ISTALA = 1

IDIRLA I 1, 2, 3 [1] O L1
x, y or z direction of the complete model
it corresponds to the main directions of the flow
useful if MODCPL > 0

5.7.5 Volume statistics

ISTALA I 0, 1 [0] C L1
activation (=1) or not (=0) of the calculation of the volume statistics related to the dispersed phase
if ISTALA = 1, the calculation of the statistics is activated starting from the absolute iteration (including the restarts) IDSTNT
by default, the statistics are not stationary (reset to zero at every Lagrangian iteration). But if ISTTIO=1, since the flow is steady, the statistics will be averaged overt he different time steps
the statistics represent the significant results on the particle cloud
always useful

SEUIL R positive real number [0.D0] O L1
every cell of the calculation domain contains a certain quantity of particles, representing a certain statistical weight (sum of the statistical weights of all the particles present in the cell). SEUIL is the limit statistical weight value, below which the contribution of the cell in term of statistical weight is not taken into account in the volume statistics (for the complete turbulent dispersion model, in the Poisson's equation used to correct the mean velocities or in the listing and post-processing outputs)
useful if ISTALA = 1

IDSTNT I strictly positive integer [1] C L1
absolute Lagrangian iteration number (includings the restarts) after which the calcu-

lation of the volume statistics is activated
useful if ISTALA = 1

NSTIST I integer $\geqslant$ IDSTNT [IDSTNT] O L1
absolute Lagrangian iteration number (includings the restarts) after which the volume statistics are cumulated over time (they are then said to be stationary)
if the absolute Lagrangian iteration number is lower than NSTIST, or if the flow is unsteady (ISTTIO=0), the statistics are reset to zero at every Lagrangian iteration (the volume statistics are then said to be non-stationary)
useful if ISTALA=1 and ISTTIO=1

NOMLAG CA string of less than 50 characters [VarLagXXXX] O L1
name of the volumetric statistics, displayed in the listing and the post-processing files. The default value is given above, with "XXXX" representing a four digit number (for instance 0001, 0011 ...)
useful if ISTALA = 1
Warning: this name is also used to reference information in the restart file (ISUIST =1). If the name of a variable is changed between two calculations, it will not be possible to read its value from the restart file

NVLSTS I $0 \leqslant$ integer $\leqslant$ NUSSTA=20 [0] O L1
number of additional user volume statistics
the additional statistics (or their cumulated value in the stationary case) can be accessed in the array STATIS by means of the pointer ILVU: STATIS(IEL,ILVU(II)) (IEL is the cell index-number and II an integer between 1 and NVLSTS)
useful if ISTALA = 1

NPST I positive integer [0] O L3
number of iterations during which stationary volume statistics have been cumulated
useful if ISTALA=1, ISTTIO=1 and if NSTIST is inferior or equal to the current Lagrangian iteration
NPST is initialised and updated automatically by the code, its value is not to be modified by the user

NPSTT I positive integer [0] O L3
number of iterations during which volume statistics have been calculated (the potential iterations during which non-stationary statistics have been calculated are counted in NPSTT)
useful if ISTALA=1
NPSTT is initialised and updated automatically by the code, its value is not to be modified by the user

TSTAT R positive real number [DTP] O L3
if the volume statistics are calculated in a stationary way, TSTAT represents the physical time during which the statistics have been cumulated
if the volume statistics are calculated in a non-stationary way, then TSTAT=DTP (it is the Lagrangian time step, because the statistics are reset to zero at every iteration)
useful if ISTALA=1
TSTAT is initialised and updated automatically by the code, its value is not to be modified by the user

5.7.6 Display of trajectories and particle movements

IENSI1 I 0, 1 [0] O L1
activation (=1) or not (=0) of the post-processing in trajectory mode
this option generates files allowing to display the trajectory of some pre-selected particles in the *EnSight6* format
always useful
Warning: this option very expensive with regards to CPU time and may generate very large files

IENSI2 I 0, 1 [0] O L1
activation (=1) or not (=0) of the post-processing in movement mode
This option generates files allowing to display the movement of some pre-selected particles in the *EnSight6* format
always useful
Warning: this option very expensive with regards to CPU time and may generate very large files

NBVIS I positive integer [NLISTE] O L1
number of particles selected for post-processing display in trajectory or movement mode
NBVIS must be lower than NBPMAX and NLISTE (set to 500 in `lagpar.h` and not to be modified)
useful if IENSI1 = 1 or IENSI2 = 1

NVISLA I strictly positive integer [1] O L1
output period for the post-processing in trajectory or movement mode
may be useful to diminish the size of the post-processing files
useful if IENSI1 = 1 or IENSI2 = 1

LISTE IA positive integers [between 1 and 500] O L1
contains the index-numbers of the particles selected for the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1

IVISV1 I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "velocity of the locally undisturbed fluid flow field" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1

IVISV2 I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "particle velocity" with the display in trajectory or movement mode
useful if IENSI1 = 1 ou IENSI2 = 1

IVISTP I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "residence time" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1

IVISDM I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "particle diameter" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1

IVISTE I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "particle temperature" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1

IVISMP I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "particle mass" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1

IVISHP I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "temperature of the coal particles" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1, if and only if IPHYLA = 2

IVISDK I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "shrinking core diameter of the coal particles" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1, if and only if IPHYLA = 2

IVISCH I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "mass of reactive coal of the coal particles" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1, if and only if IPHYLA = 2

IVISCK I 0, 1 [0] O L1
associates (=1) or not (=0) the variable "mass of char of the coal particles" with the display in trajectory or movement mode
useful if IENSI1 = 1 or IENSI2 = 1, if and only if IPHYLA = 2

5.7.7 Display of the particle/boundary interactions and the statistics at the boundaries

IENSI3 I 0, 1 [0] C L1
activation (=1) or not (=0) of the recording of the particle/boundary interactions in PARBOR, and of the calculation of the statistics at the corresponding boundaries, for post-processing (*EnSight6* format)
By default, the statistics are non-stationary (reset to zero at every Lagrangian iteration). They may be stationary if ISTTIO=1 (*i.e.* calculation of a cumulated value over time, and then calculation of an average over time or over the number of interactions with the boundary)
always useful

NSTBOR I strictly positive integer [1] O L1
number of absolute Lagrangian iterations (including the restarts) after which the statistics at the boundaries are considered stationary and are averaged (over time or over the number of interactions)
If the number of absolute Lagrangian iterations is lower than NSTBOR, or if ISTTIO=0, the statistics are reset to zero at every Lagrangian iteration (non-stationary statistics)
useful if IENSI3=1 and ISTTIO=1

SEUILF R positive real number [0.D0] O L1
every boundary face of the mesh undergoes a certain number of interactions with particles, expressed in term of statistical weight (sum of the statistical weights of all the particles which have interacted with the boundary face). SEUILF is the limit statistical weight value, below which the contribution of the face is not taken into account in the statistics at the boundaries for post-processing
useful if IENSI3=1

INBRBD I 0, 1 [1] O L1
activation (=1) or not (=0) of the recording of the number of particle/boundary interactions, and of the calculation of the associated boundary statistics.
INBRD = 1 is a compulsory condition to use the particulate average IMOYBR = 2
the selection of the type of interactions that are to be recorded is specified in the subroutine `uslabo`
useful if IENSI3=1

IFLMBD I 0, 1 [0] O L1
activation (=1) or not (=0) of the recording of the particulate mass flow related to the particle/boundary interactions, and of the calculation of the associated boundary statistics
the selection of the type of interactions that are to be recorded is specified in the subroutine `uslabo`
INBRD = 1 is a compulsory condition to use IFLMBD=1
useful if IENSI3=1 and INBRBD=1

IANGBD I 0, 1 [0] O L1
activation (=1) or not (=0) of the recording of the angle between a particle trajectory and a boundary face involved in a particle/boundary interaction, and of the calculation of the associated boundary statistics
the selection of the type of interactions that are to be recorded is specified in the subroutine `uslabo`
useful if IENSI3=1

IVITBD I 0, 1 [0] O L1
activation (=1) or not (=0) of the recording of the velocity of a particle involved in a particle/boundary interaction, and of the calculation of the associated boundary statistics
the selection of the type of interactions that are to be recorded is specified in the subroutine `uslabo`
useful if IENSI3=1

IENCBD I 0, 1 [0] O L1
activation (=1) or not (=0) of the recording of the mass of coal particles stuck to the wall due to fouling, on the boundary faces of the IENCRL interaction type
useful if IENSI3=1, IPHYLA=2, IENCRA=1, and if there is at least one boundary face of the IENCRL interaction type

NUSBOR I positive integer [0] O L1
number additional user data to record for the calculation of additional boundary statistics in PARBOR
useful if IENSI3=1

NOMBRD CA string of less than 50 characters [see `uslag1`] O L1
name of the boundary statistics, displayed in the listing and the post-processing files
useful if IENSI3=1
Warning: this name is also used to reference information in the restart file (ISUIST =1). If the name of a variable is changed between two calculations, it will not be possible to read its value from the restart file

IMOYBR IA 0, 1, 2 [0 , 1 or 2] O L1
the recordings in PARBOR at every particle/boundary interaction are cumulated values (possibly reset to zero at every iteration in the non-stationary case). They must therefore be divided by a quantity to get boundary statistics. The user can choose between two average types:
= 0: no average is applied to the recorded cumulated values
= 1: a time-average is calculated. The cumulated value is divided by the physical duration in the case of stationary averages (ISTTIO=1). The cumulated value is divided by the value of the last time step in the case of non-stationary averages (ISTTIO=0), and also in the case of stationary averages while the absolute Lagrangian iteration number is inferior to NSTBOR
= 2: a particulate average is calculated. The cumulated value is divided by the number of particle/boundary interactions (in term of statistical weight) recorded in PARBOR(NFABOR,INBR). This average can only be calculated when INBRBD=1. The average is calculated if the number of interactions (in statistical weight) of the considered boundary face is strictly higher than SEUILF, otherwise the average at the face is set to zero
only the cumulated value is recorded in the restart file
useful if IENSI3=1

NPSTF I positive integer [0] O L3
number of iterations during which stationary boundary statistics have been cumulated
useful if IENSI3=1, ISTTIO=1 and NSTBOR inferior or equal to the current Lagrangian iteration
NPSTF is initialised and updated automatically by the code, its value is not to be modified by the user

NPSTFT I positive integer [0] O L3
number of iterations during which boundary statistics have been calculated (the potential iterations during which non-stationary statistics have been calculated are counted in NPSTFT)
useful if IENSI3=1
NPSTFT is initialised and updated automatically by the code, its value is not to be modified by the user

TSTATP R positive real number [DTP] O L3
if the recording of the boundary statistics is stationary, TSTATP contains the cumulated physical duration of the recording of the boundary statistics
if the recording of the boundary statisticss is non-stationary, then TSTAT=DTP (it is the Lagrangian time step, because the statistics are reset to zero at every time step)
useful if IENSI3=1

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7 Appendix 1 : automatic validation procedure

7.1 Introduction

This document is the practical user guide for the autovalidation procedure associated with *Code_Saturne* version 1.3.2. The aim of this document is to guide the user through all the steps necessary for the running and the user-understanding of the autovalidation procedure. The guide describes the selected test cases, the modifiable settings and the procedure to add a case in the reference base.

The procedure is written in python language and a XML file containing the data settings is necessary.

7.2 Practical informations on the procedure

This procedure aims to run automatically all the selected cases and to compare the obtained results with those of the reference base. All the comparisons are summarized in a report file. If the discrepancies between the reference and the test overpass a determined tolerance, the procedure creates an EnSight part containing the variable differences.

For each test cases, the detailed actions are the following:

- preparation of the study with the *cree_sat* utility,
- copy of all the necessary files (meshes, XML data file, user fortran files) from the reference base,
- execution of the case with the *runcase* utility,
- comparison between the reference results and the test results,
- update of the report file.

First, an empty directory named BASETEST is generated by the user. In this directory, the command to launch the script is the following:

autovalid -f [xml file name] [-d [tmp directory]]

where *xml file name* is the data file containing the settings necessary to the autovalidation. The reference base has to be easily updatable. The user has to copy this file, initially associated to the directory BASEREF, in the directory BASETEST in order to modify it (for example, if the user doesn't want to execute all the tests or if he wants to compare only some variables).

7.3 Directories architecture

The typical architecture is given in the following section:

- a directory BASEREF containing all the reference studies (five elementary tests GRADIENT and LAPLACIEN) and the XML data file *autovalid.xml*,
- the user has to create a directory BASETEST and to copy the XML data file *autovalid.xml* in this directory before launching the script,
- a directory Autovalid containing all the python source files.

7.4 Validation base

The selected cases in the reference directory are:

- GRADIENT : elementary tests of gradient calculation using the different methods proposed by *Code_Saturne*,
- LAPLACIEN : resolution of a laplacian equation.

7.4.1 Elementary tests : gradient calculations

The elementary tests are performed on a cubical mesh composed by hexahedrons and tetrahedrons with non-conforming merging. The mesh is generated using Simail-6.4 mesher (file with extension *.des*).

All the tests are contained in the fortran file *testel.F* called by the fortran file *caltri.F*. To activate the elementary tests, we use the existing parameter IVERIF in the main program *cs_main.c*. IVERIF is initialised to -1 (no action). If IVERIF takes the value 0, there is no difference with the standard version. If IVERIF > 0, *testel.F* will be called with :

- IVERIF = 1: IMRGRA = 0
- IVERIF = 2: IMRGRA = 1
- IVERIF = 3: IMRGRA = 2
- IVERIF = 4: IMRGRA = 3
- IVERIF = 5: IMRGRA = 4

A new keyword ARG_CS_VERIF refering to IVERIF is added in the universal launch script *lance*, so that the command line is: *cs12.exe -v ARG_CS_VERIF*.

The test case consists in calculating the gradient of sin(x+2y+3z) with the different methods implemented in *Code_Saturne* (boundary conditions are treated with Dirichlet condition). We compare the result to the reference solution (not to the exact solution).

7.4.2 Laplacien calculation

The mesh is the same as for the previous elementary tests.

The case consists in the resolution of a stationary equation without convection terms for a passive scalar. The source term and Dirichlet boundary conditions are specified so that the solution is sin(x+2y+3z). The source term is imposed in the fortran file *ustssc.F*. We compare the result with the reference solution (not with the exact solution).

7.5 Architecture description

In the directory Autovalid, the user finds all the python source files necessary to the execution of the procedure. The main file *autovalid* runs the autovalidation and manages the general printouts.

7.5.1 Python files in the modules directory

All the python files are listed here:

- *Common.py*: this file contains the global variables (XML file name, reference version, reference path, temporary directory and local directory),
- *CommandLine.py*: this file manages the command line usage,
- *Parser.py*: this file defines the parser class which loads and reads the XML data file,

- *Study.py*: this file defines the study class which contains case objects,
- *Case.py*: this file defines the case class which contains the launch script and the listing and chrono comparisons,
- *Listing.py*: this file defines the listing class which contains minima/maxima variables and clippings,
- *Chrono.py*: this file defines the chrono class which contains a list of values and creates, if necessary, a part EnSight (if tolerance > specified value).

7.5.2 XML file description

The XML file contains all the data to run the different cases. It is important to note the definitions of the following attributes:

- *label* refers to the name of the study, the name of the case, the name of the variable or the name of the post-treatment script,
- *status* is 'on' or 'off' to activate or not the action,
- *compute* is 'on' or 'off' to run or not the calculation,
- *tolerance* is the maximum allowed value for the norm of the variable X defined by

$$\frac{|X_{Ref} - X_{Test}|}{|X_{max_{Ref}} - X_{min_{Ref}} + \varepsilon|}$$

.

An example of XML data file is given below:

```
<?xml version="1.0"?>
<autovalid name="Validation Saturne V1.3">
  <referencepath>/home/vit/SATURNE/BASEREF</referencepath>
  <referenceversion>SaturneV1.3</referenceversion>

  <study label='LAPLACIEN' status='on'>
    <variable label='passif' status='on'>
      <tolerance>0.1</tolerance>
    </variable>
    <variable label='Pression' status='on'>
      <tolerance>0.1</tolerance>
    </variable>
    <variable label='VitesseX' status='on'>
      <tolerance>0.1</tolerance>
    </variable>

    <case label='CAS1' status='on' compute='on'>
      <post label='depou_elargb' status='off'> </post>
    </case>

    <case label='VERIF' status='on' compute='on'>
      <post label='depou_elargb' status='off'> </post>
    </case>

    <case label='2PROCS' status='on' compute='on'>
```

```
      <post label='depou_elargb' status='off'> </post>
      <nproc>2</nproc>
    </case>
  </study>

</autovalid>
```

Note : If *status* is 'on' and *compute* is 'off', we compare listing files and chrono files but if there isn't result available, *compute* becomes 'on'.

7.5.3 To add a new study

To add a new study in the reference base, the user has to create and run a calculation in the directory BASEREF. He also has to add the following typical section in the XML data file:

```
<study label='GRADIENT' status='on'>
  <variable label='gradient' status='on'>
    <tolerance>0.1</tolerance>
  </variable>

  <case label='CAS1' status='on' compute='on'>
  </case>
</study>
```

For example, this previous sequence means that the user wants to run (compute is 'on') and compare the variable 'gradient' with a tolerance 0.1 for the case CAS1 of the study GRADIENT.

7.5.4 Report files

There are three kinds of report file :

- *report.txt*: this general file contains just OK, NOK, 'Execution error' or 'Compilation error' for each case of each study,
- *STUDY_listing.report*: this file depends on the study and contains the listing files comparison for each selected variable at the last time step (min/max values, min/max norms, min/max clippings),

$$Norm_{X_{max}} = \frac{|X_{max_{Ref}} - X_{max_{Test}}|}{|X_{max_{Ref}} - X_{min_{Ref}} + \varepsilon|}$$

$$Norm_{X_{min}} = \frac{|X_{min_{Ref}} - X_{min_{Test}}|}{|X_{max_{Ref}} - X_{min_{Ref}} + \varepsilon|}$$

- *STUDY_chrono.report*: this file depends on the study and contains the chrono files comparison for each selected variable at the last time step (maximum difference, mean difference and norm),

$$\delta_{max} = max|X_{Ref} - X_{Test}|$$

$$\delta_{mean} = \frac{\sum |X_{Ref} - X_{Test}|}{Nb_{values}}$$

$$Norm = \frac{\delta_{max}}{|X_{max_{Ref}} - X_{min_{Ref}} + \varepsilon|}$$

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